YEARBOOK

1983-84

CENTRAL RESEARCH INSTITUTE for PHYSICS

OF THE HUNGARIAN ACADEMY OF SCIENCES

MTA KFKI

1983-84

KFKI

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MTA • Központi Fizikai Kutató Intézet

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P R E F A C E

It is a tradition of our research centre to publish, every second year, a biennial report as a means of informing our friends all over the world about our activities and results.

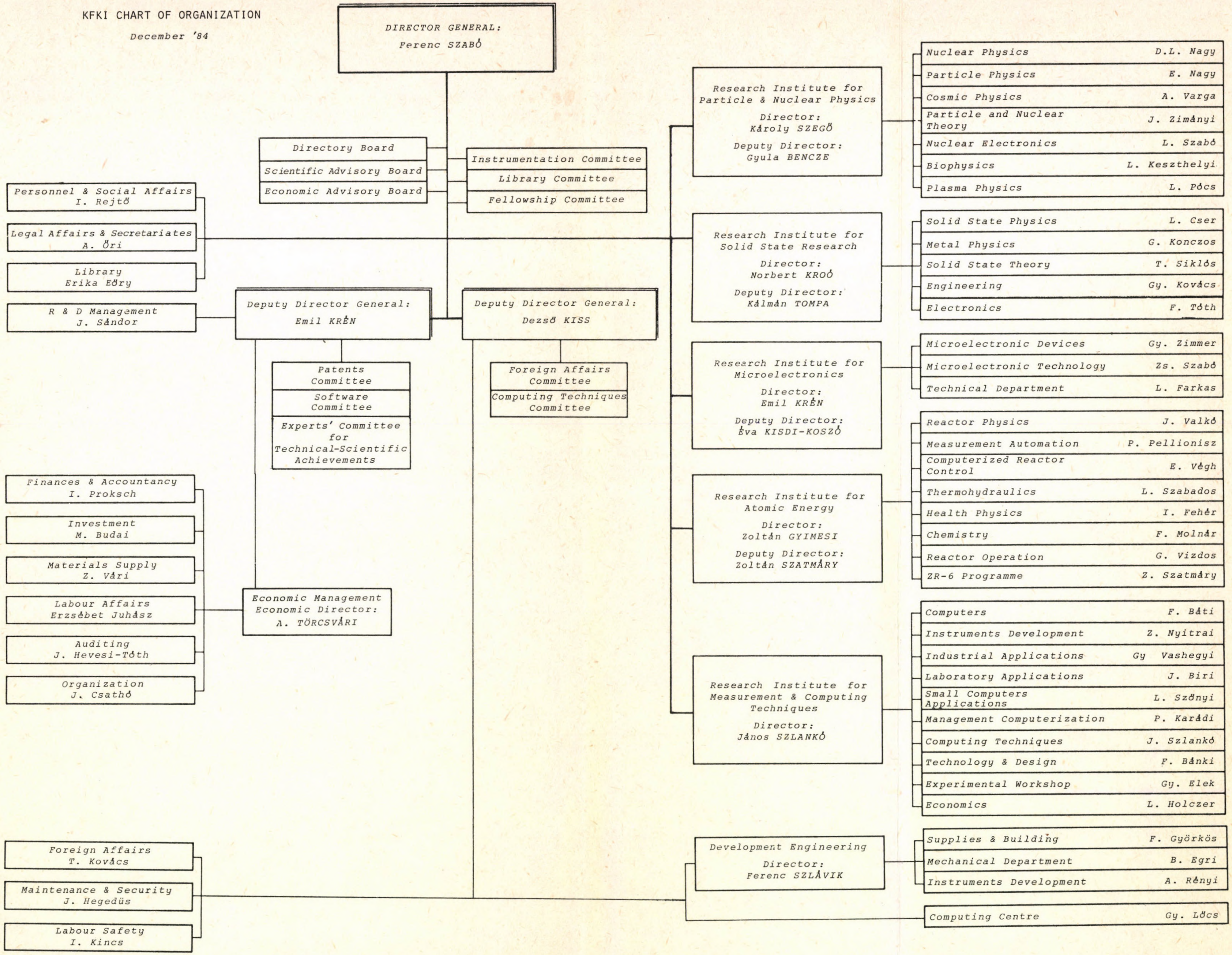
The general structure of the present yearbook is similar to the previous one. The activities of the institutes of the research centre are again covered by general progress reports together with more detailed descriptions of some outstanding results.

We do hope you will find this booklet useful as a means of orientation. Should you wish to obtain more details about any aspect of our research centre or our results in any of the specialized fields, do not hesitate to contact us; we shall be pleased to let you have the relevant information.

Director General

KFKI CHART OF ORGANIZATION

December '84



RESEARCH INSTITUTE FOR PARTICLE AND NUCLEAR PHYSICS (RMKI)

The organization of our research centre reflects a certain classification of physics research into main branches. The development of science, however, does not usually follow rigid borderlines. As a result, scientific activity is much more versatile than the administrative framework.

The Research Institute for Particle and Nuclear Physics therefore is currently conducting research in the following main fields:

a) particle physics;
b) nuclear physics;
c) space physics;
d) applied nuclear physics and materials science;
e) fusion research.

The scientific profile of the institute is essentially determined by the dominance of basic research.

In the following short description of our activities, the results will be grouped according to the logic of science rather than organizational aspects.

THEORETICAL PARTICLE AND NUCLEAR PHYSICS, GENERAL RELATIVITY AND ASTROPHYSICS

The main problem in present day particle physics theory is to understand the strong interaction. It is generally believed that the key to the problem lies in the theory of gauge fields. Several aspects of this theory have been studied by our staff. The successful work of former years has been continued in lattice quantum-chromodynamics (QCD). Results have been obtained in SU (3) lattice gauge theory concerning the string tension, the deconfinement phase transition in the presence of quarks and the rotational symmetry of the SU (3) potential. In addition, new methods to find satisfactory solutions of QCD have been explored. The method of microcanonical simulation, which has been successfully applied to study fermionic systems, is one such method. The renormalization group, especially the β-function, has also obtained importance in the study of SU (3) lattice gauge theories and two-dimensional non-linear σ-model.

Another, closely related subject has been the search for magnetic monopole solutions in classical gauge field theories. Such solutions always exist in spontaneously broken gauge theories, and these theories seem now to give the only chance for a unified description of the various interactions. Starting from the simplest cases, systematic work has led to a method which gives the most general n-monopole solutions. Within the framework of unified theories, we have been successful in dimensional reduction and spontaneous compactification.

Some work has been directly related with phenomenology. For example, radiative corrections to the charged weak form factors in hyperon semi-leptonic decays have been calculated. In addition, we have studied the description of hadron-hadron multiparticle processes in the additive quark model.

In low energy nuclear physics the main theoretical investigations can be characterized as the application of methods of exact nonrelativistic scattering theory to various nuclear problems.

Along this line the exact N-body scattering theory was used to clarify certain aspects of direct nuclear reactions.

The Faddeev equations were used for further investigation of the three-nucleon system; particularly, a detailed study of the dependence of triton properties on the deuteron wave function was performed. An approximate way of inclusion of the Coulomb force into three-body calculations was suggested and tested for the d-α case.

In a systematic search for promising applications of separable interactions, an exactly soluble model for the quantum dynamics of a particle in the field of two classically moving potentials was proposed and applied for light particle emission and transfer in heavy ion collisions.

A new method was found for the compact solution of the fully off-the-energy-shell Lippman-Schwinger equation.

The description of the interaction of fast neutrons with nuclei was attempted in the framework of a cascade model; Monte-Carlo calculations were performed to reproduce the excitation functions and the neutron spectra for neutron induced reaction on the Ta nucleus.

In the field of relativistic heavy ion physics efforts were centred on the description of the properties of the exotic forms of matter formed in the reactions and on the search for signatures showing the formation of that very hot and dense matter.

It was shown that the anisotropy of the momentum distribution of the participant nucleons enhances the probability of the formation of pion condensate.

A strong increase in the produced K meson/π meson ratio is predicted as a signature for the formation of the quark-gluon plasma.

In the theory of general relativity, our research has continued for solutions of Einstein's gravitational equations. Such exact solutions find significant applications in relativistic astrophysics (black holes, quasars). Using Lyapunov functional techniques, it has been shown that the Robinson-Trautman model of rotation-free gravitational collapse yields asymptotically the Schwarzschild black hole solution. Space-times sharing the conformal symmetry property of the Schwarzschild solution have been found. In addition, by using a suitable combination of the theory of Killing vectors with Newman-Penrose equations, a variety of exact vacuum space-times was obtained. Bounds on the matter distribution that are imposed by relativistic causality have been discovered.

Among the applications to cosmology, models of the early Universe and some cosmological symmetry principles have been considered. Progress was achieved in the understanding of the hydrodynamical and thermodynamical properties of the relativistic continuum.

Our interest in the proposed generalizations of relativity to include quantum effects is concentrated mostly on Penrose's twistor theory. Such a description of curved spaces is a largely unexplored area, and efforts have been made at a twistor description of particles with rest mass. Another attempt has been made at deducing the structure of space-time from quantum principles. Part of our research has been carried out in collaboration with the University of Pittsburgh, in the framework of a scientific exchange programme.

PARTICLE PHYSICS

The European Muon Collaboration (EMC) in which a team of the Particle Physics Department participates, has continued the high precision determination of the quark momentum distributions in the nucleon and the detailed study of the hadronic final state in muoproduction.

It has been discovered that the quark momentum distribution in the nucleon depends on the nucleus in which the nucleon is embedded. This phenomenon, widely cited in the literature as the *EMC-Effect*, came as a great surprise and has far-reaching consequences. The main message is that a full description of the nucleus cannot be given only in terms of the nucleons. It is necessary to go beyond that level, presumably to the quark level.

The EMC has studied in great detail the hadronic final states in muoproduction both in the forward direction (high statistics) and in the 4π solid angle. In this latter case a streamer chamber with a vertex spectrometer has been added to the forward spectrometer and the pictures taken by the streamer chamber were measured in different laboratories, including the KFKI. Detailed distributions of the identified final state hadrons produced by different target materials have been obtained for charged and for some of the neutral particles (Λ^o, K^o, ρ^o, J/Ψ), and the asymmetry of the production azimuthal angle predicted by QCD has been verified. These results gave an essential contribution to the understanding of the muoproduction reaction mechanism and of the EMC-Effect.

The NA-4 group has run a dedicated experiment in order to verify the EMC-Effect on different target nuclei. Good agreement has been obtained with the original result of the EMC.

Progress has been achieved in the construction of the L-3 detector devoted to study electron-positron annihilation at extremely high energies using the future LEP Collider to be built at CERN. This work is being performed in a world-wide collaboration led by the Nobel Laureat Professor Samuel C.C. Ting including institutions from the US, USSR, Eastern and Western Europe as well as from China. The primary goal of the experiment is to provide detailed information on the electroweak theory and to perform a systematic search for the scalar Higgs particles necessary for the mechanism of the spontaneous symmetry breaking. The Budapest group is participating in the design of the electromagnetic calorimeter and has made a significant contribution to the development of the necessary software tools, which enables the simulation of the complex electromagnetic cascade processes on large computers.

A team of our particle physicists has continued the RISK spectrometer experiment performed at JINR. The aim of this research is the study of hadron-nucleus interactions at 40 GeV in a wide region of the periodic table ranging from lithium to lead. The charged particle multiplicites, the normalized mean multiplicities of negative particles have been investigated in π^-, K^- and $\bar{p}$ interactions with nuclei. A universal description of multiplicity distributions of negative particles was given, which was in good agreement with the experimental data. The investigations of the characteristics of the momentum, angular and rapidity distributions of charged secondaries with high transverse momentum trigger are in progress.

COSMIC PHYSICS AND SPACE RESEARCH

The scientific cosmic physics department has continued its work in the field of classical cosmic ray research and in space physics. In particular we have studied the interaction of energetic charged particles with interplanetary plasma and the interaction of the solar wind with non-magnetic bodies in the solar system.

In cooperation with the Lebedev Physical Institute, Moscow, the measurement of primary cosmic radiation of energy around 10^{14} eV were continued and the analysis of data to determine the global anisotropy is in progress.

Cosmic muons of energies $\sim 10^{11}$ eV were registered by the underground muon telescope at Budapest in order to explore the solar modulation of galactic cosmic rays.The intensity variations measured imply that the solar diurnal vector returned to the 18 hour phase in 1983. The correlation of the daily variation in sidereal time, with different interplanetary magnetic sectors favours the idea of a pitch angle distribution, in contradiction to the density gradient model.

In the field of modulation theory, the method of calculating energy losses along regular trajectories in a model interplanetary magnetic field was extended to describe the Forbush effects at high rigidities. In the simple field model adopted, the gross features of the events were well reproduced.

Cosmic ray observations at lower energies were carried out aboard space probes. In collaboration with the Imperial College, London, measurements of 35-1000 keV protons made by the ISEE-3 spacecraft were analysed. The bidirectional pitch angle distributions found in association with quasiperpendicular interplanetary shocks support the idea of the formation of a magnetic bottle prior to the shock passage. Based on the intensity measurements of 10 MeV protons and 0.5 MeV electrons on board the space probes Helios 1, 2 and Prognoz 6, a multispacecraft study of two, flare associated particle events was performed and the interplanetary and coronal propagation parameters were determined.

In connection with planet Venus using Pioneer Venus Orbiter magnetic field observations between 1979 and 1981 the location of the bow shock around the planet was determined. The ultra low frequency (10-40 sec period) magnetic field fluctuations in the magnetosheath were traced along stream lines. It was suggested that ionopause disturbances may be caused by convection of turbulent magnetic fields from the subsolar bow shock. Another new result is that magnetic field overshoots occur behind quasi-parallel shock and are supercritical, while the amplitude increases with increasing Mach number. In order to test the validity of the gas dynamic treatment, which neglects magnetic field in the shock structure and the flowing plasma, the proper Mach number and the ratio of specific heats were determined. The Venus bow shock was found to be much farther away than the gas dynamic model predicts.

In the field of cometary physics, gas dynamic calculations were performed to model the cometary atmosphere. Terminal velocities of dust particles were obtained using a realistic dust size distribution. Examining particle trajectories in a cometary coma under the influence of solar light pressure and accelerating gas, the dust density distribution and the subsolar distance were calculated. The study was extended by including the effect of electrostatic charging of the dust in a simplified magnetic field configuration, and consequences on the in situ dust experiments were examined.

Polarisation electric fields in the cometary environment were studied and shown to influence both the cometary plasma and the fine cometary dust. The ambipolar electric field turned out to be important in the outer regions where the abruptly increasing electron temperature gives rise to an electric field that first decelerates (up to 500 km) and then increasingly accelerates (above 1500 km) the ion flow. The possibility of an inner shock due to the deceleration was also studied.

To the coupled dusty hydrodynamic equations describing the cometary coma, time-dependent solutions that represent spherically symmetric expansion of neutral gas were found. The time evolution of a cometary outburst was also modeled, which shows the generation of a slow disturbance in addition to the blast wave.

NUCLEAR PHYSICS

A team of our nuclear physicists performed experiments with 300–550 MeV neutrons and 1 GeV protons in order to understand the physical basis of inclusive production of fast particles at intermediate energies. In a collaboration with scientists at Freiburg University an experiment was performed at the Swiss Institute for Nuclear Research (SIN) in which neutrons were incident on ^{12}C nuclei. Charged particle spectra were measured at different angles ranging from 73^o to 165^o. The energy spectra of protons, deuterons and tritons were similar to those observed in proton induced reactions, and the integrated cross section of protons was found to be about 40% of the cross section measured with primary protons. This suggests the importance of the role of simple reaction mechanisms involving only a few target nucleons.

In collaboration with the Leningrad Institute for Nuclear Physics proton-nucleus collisions have been studied at 1 GeV. Charged particle spectra were measured at large backward angles on different calcium isotopes. A definite isotopic effect was observed in the particle production.

Preequilibrium phenomena were investigated in E/A=35 MeV ^{14}N-ion collisions with ^{165}Ho, Ni and ^{12}C nuclei measuring the neutron emission in coincidence with light fragments. The measurements were carried out at the MSU K500 superconducting cyclotron in collaboration, sponsored by MTA-NSF contract, with the Eötvös University, the KFKI and MSU. The neutron distributions reveal significant contributions of preequilibrium and sequential resonance neutron emission.

In the field of the nuclear fission, the energy distribution of the prompt fission neutrons was measured for the spontaneously fissioning ^{252}Cf, as well as for the thermal fission of ^{233}U, ^{235}U and ^{235}U.

Special attention was paid to the determination, by Monte Carlo calculations, of the absolute neutron detection efficiency. It was found that the spectra can be described well by Maxwellian distributions.

Investigations have been started in the field of the (HI,xn) reactions. The angular and energy distributions of neutrons have been measured in the reactions Ti+^{12}C, Ti+^{16}O and Ti+^{20}Na at the Dubna Institute.

Studies of the fragmented $1g_{9/2}$ IARs in ^{51}Mn and ^{53}Mn were completed. The identification of the resonance fragments was helped by their relative strong decay to the second excited 4^+ levels of the target nuclei, ^{50}Cr and ^{52}Cr. Fine structure analyses were performed in all open channels. The results show that the fragmentation patterns are different in the different channels in disagreement with theoretical suggestions.

MATERIALS SCIENCE, USING NUCLEAR METHODS

According to the nuclear technique used, the main research fields have been (i) Mössbauer spectroscopy of solids and amorphous systems, (ii) positron annihilation studies in solids, and (iii) exotic atoms research.

Detailed Mössbauer measurements have been performed at 4.2 K on a series of crystalline compounds, containing the ferrous hexaquo complex, in magnetic fields up to 5 T. The results have been interpreted in terms of a T_{2g} ligand field model for which normal distortions of the water octahedron were used as parameters.

Systematic work on ferrous halogenide aqueous solutions has resulted in new information on the conditions for the formation of the vitreous state. In ferrous chloride, bromide and iodide solutions, a vitreous state is formed whereas in ferrous fluoride solutions it is not observed. Mössbauer studies were performed in parallel with differential thermal analysis (DTA) of the samples: the DTA curve of FeF_2 does not indicate any glass transition *(Fig. A-1)*.

Another intensively studied problem was the location of impurities in semiconductors. With regard to the location of Te in epitaxially regrown Si layers, Mössbauer studies showed a quadrupole doublet in annealed ^{125m}TeSi. This indicates that at least 80% of the Te atoms have a symmetry that is lower than expected cubic symmetry.

We have analyzed through electronic structure investigations, based on a model of an impurity atom trapped close to a substitutional site adjacent to a vacancy, the nuclear quadrupole interactions of ^{125}Te and ^{129}I implanted in a number of group IV and III-V semiconductors (GaAs, GaSb, GaP, InP). The results for these impurity systems support the model.

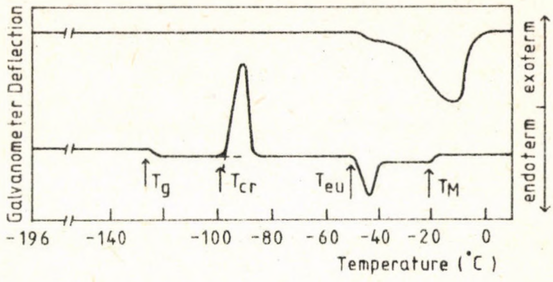


Fig. A-1

DTA curves of FeF_2 (upper) and FeI_2 (lower) aqueous frozen solutions. T_g: glass transition-, T_{cr}: crystallisation-, T_{eu}: eutectic melting-, T_m: ice melting temperatures

Al_2O_3 and $LiNbO_3$ samples implanted by ^{57}Co and ^{57}Fe were examined by Mössbauer spectroscopy. The emission and absorption (CEMS) measurements indicate that ^{57}Co and ^{57}Fe could find similar lattice positions and also that highly ionized iron states do not form in either case after implantation.

A new phenomenon, viz. a long-lived non-equilibrium population of the Zeeman sublevels of the ^6S ground state of Fe^{3+} ions, has been found after the electron capture of ^{57}Co in frozen aqueous solution of $^{57}CoCl_2$, $Fe(BF_4)_2 \cdot 6H_2O$:^{57}Co, $LiNbO_3$:^{57}Co and $LiTaO_3$:^{57}Co. After the Auger process and the following recombination cascade the anomalous population of these sublevels results in the appearence of sharp anomalous lines in the emission Mössbauer spectrum (cf. *Fig. A-2*). The systematic investigation of the temperature- and magnetic field dependence of the line intensities showed that those are proportional to the initial populations of the Zeeman sublevels.

The intensities of the anomalous lines are extremely sensitive to the direction of the crystal field which is a direct evidence for the role of non-ground terms of Fe^{3+}.

Iron-zirconium amorphous and crystalline alloys were extensively studied by Mössbauer spectroscopy and positron lifetime measurements as well. The crystallization process of an amorphous $Zr_{75}Fe_{25}$ sample was investigated. The positron lifetime is higher in the amorphous state, but it depends very sensitively on the defect concentration as well. The hydrogen desorption process of $Zr_3FeH_{5.5}$ sample was followed by both

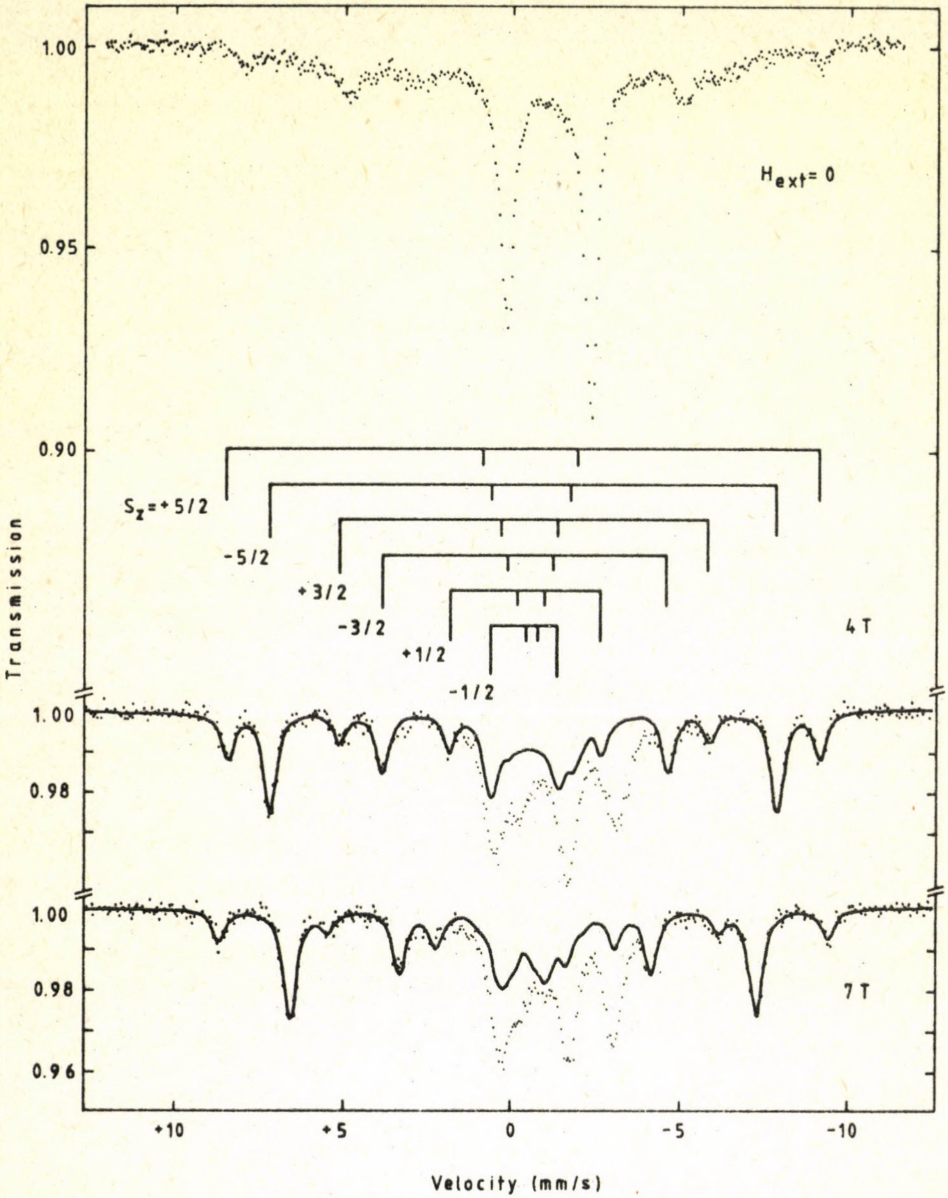


Fig. A-2

Mössbauer emission spectra of $LiNbO_3$:^{57}Co single crystals at 4.2 K in various longitudinal magnetic fields H⊥c methods. The two most important features observed are the appearance of the metastable Zr_3Fe phase and the hydrogen induced decomposition into Fe_2Zr, Zr_3Fe and Zr at 600 ^{o}C. A linear dependence of the isomer shift on the hydrogen content was found and it was attributed both to lattice relaxation as a consequence of the H desorption and to H induced changes in the electronic structure. The higher positron lifetimes suggest a defect-rich structure before the metastable phase appears.

We succeeded in charging amorphous $Zr_{76}Fe_{24}$ with hydrogen by electrolitical method. Mössbauer spectra of the pure amorphous and the hydrogenized sample are shown in *Fig. A-3*.

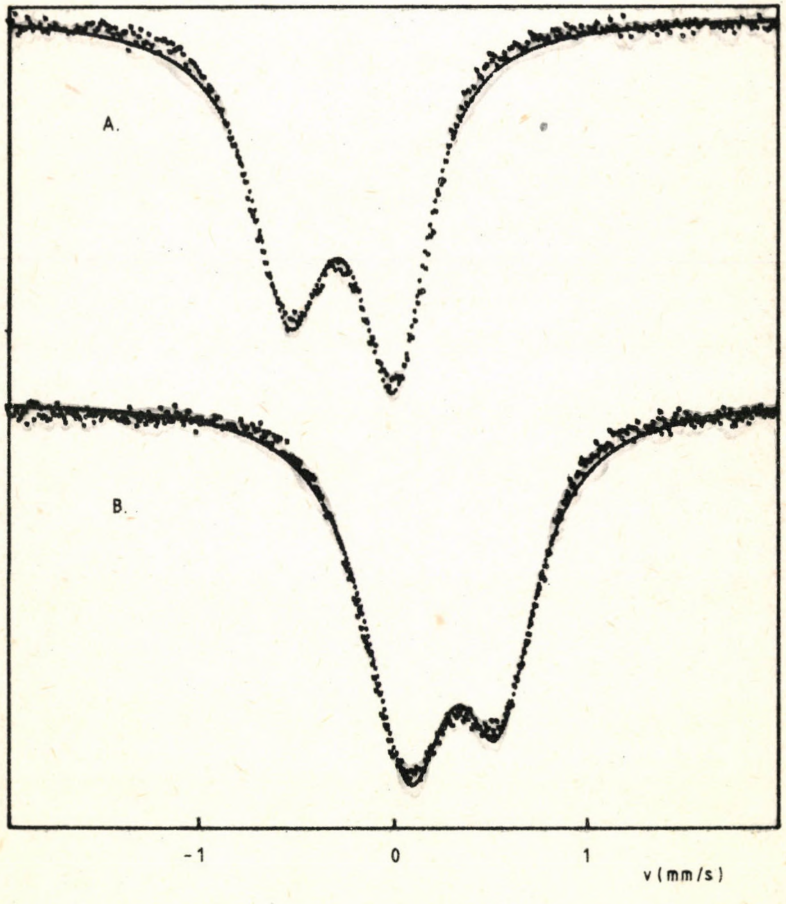


Fig. A-3

The Mössbauer spectra of a-$Zr_{76}Fe_{24}$ without (A) and with hydrogen saturation (B)

Positron annihilation measurements were performed on the ordered β-Hume-Rothery phase of PdIn alloy (B2 structure) and on Pd-rich and In-rich phases, in thermal equilibrium and after quenching. On the off-stoichiometric samples, using the positron lifetime technique, the existence of constitutional defect-positron (In-rich side) and antistructure atom-positron (Pd-rich side) bound states were demonstrated, and the lifetime of these structures were determined. The measurements on the quenched, stoichiometric sample show that beside the Pd vacancies also In vacancies exist.

Systematic experimental study has been performed on the atomic capture of stopped negative pions in binary mixtures of ^3He with Z= ^4He, Ne, Ar, Kr, Xe, N_2, O_2, CO_2 and SF_6 in gas state. We determined the concentration and atomic number dependence of the Z/^3He capture ratio. The influence of molecular structure on the nuclear capture probability of stopped negative pions has been observed by comparing the π^0 gamma -spectrum from π^- mesons stopped in HD and in H_2+D_2 gas. Various models of atomic capture of negative mesons were tested against 321 experimental Coulomb-capture ratios measured in binary chemical systems and shown to be inadequate to predict or describe the experimental data. A systematic analysis was performed of the possible elementary processes which determine the fate of negative pions stopped in hydrogen-containing samples. This was done with a phenomenological description in conjunction with the available experimental information on pion capture by hydrogen in gas mixtures.

An investigation is underway at TRIUMF of formation rates of ddμ and pdμ molecules in gaseous targets of hydrogen isotopes at various temperatures. The formation of the muonic molecules is signalled by nuclear fusion, either $d+d \rightarrow {}^3He+n$ or $d+p \rightarrow {}^3He+\gamma$, and the fusion neutrons and gamma-rays are detected using the electron from the muon decay as trigger.

An experiment on the effect of hydrogen bonds on pion capture by protons in ordinary and "heavy" methanol (CH_3OH, CD_3OH and CH_3OD) in solid, liquid and supercritical phases was performed and the capture probabilities were determined.

CONTROLLED FUSION RESEARCH AND PLASMA PHYSICS

Our fusion research was continued along the main lines followed in the previous years:

- investigation of physical processes in hot plasmas, mainly in tokamak devices;
- plasma-wall interaction studies;
- development of new plasma-diagnostic methods and devices.

In the field of plasma physics, the following main results were achieved.

The ion temperature of the plasma in the MT-1 tokamak was derived from the energy distribution of emitted neutral atoms, measured by means of a newly installed five-channel electrostatic analyser. *Fig. A-4* shows a typical energy distribution curve in the case of normal tokamak discharges, *Fig. A-5* (U_{loop}=4 Volts, I_{plasma}=25 kA). The spectrum of the emitted atoms in the high energy range (E>300 eV) can be described by a Maxwellian distribution with a temperature of about 130 eV.

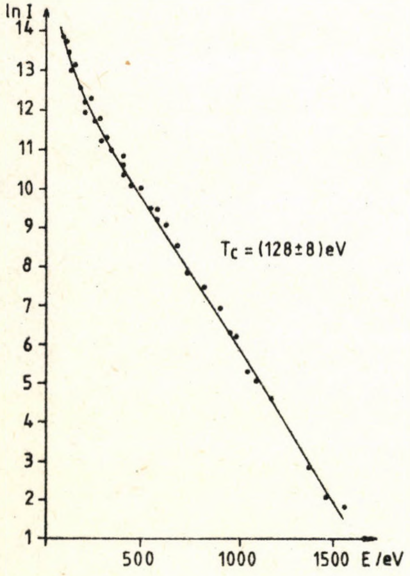


Fig. A-4

Ion temperature measured in a wide range of energy in case of a typical plasma discharge

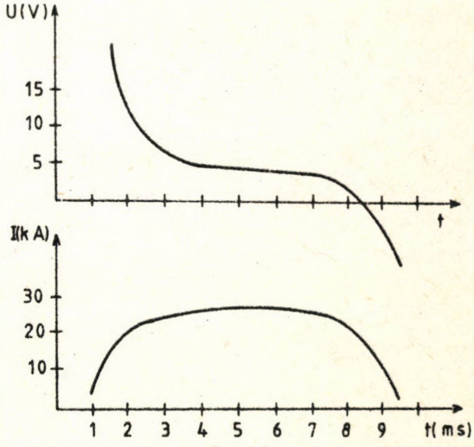


Fig. A-5

Loop voltage and plasma current for a typical discharge on the MT-1 tokamak

For the investigation of the spatial density distribution of neutral atoms in the plasma a numerical model and a computer code based on that model have been developed. The program calculates the distribution from the integral form of the Boltzmann transport equation, taking into account charge-exchange, recombination and ionization processes. Also the energy spectra of the emitted neutrals can be calculated.

An extensive study of the fluctuations occuring in the soft X-ray radiation of the tokamak plasma, has identified several characteristic regimes. A distinct feature, called the giant sawtooth oscillation, of one of these regimes is that the current signal shows jumps in correlation with the modulation of the soft X-ray radiation. Recently, a phenomenological model of the fluctuation has been developed. The model provides us with solutions which show grouping of the faster sawtooth oscillations into larger modulational patterns.

In the field of the plasma theory the non-linear phenomena in the particle transport, the magnetic field splitting and the stochastic processes have been investigated. The Gibbs phenomenon has been treated in generalized Padé approximation, and with the aid of some rational approximants the Gibbs constants have been determined. In addition, the steepness of the rational approximants has been calculated.

Within the scope of the collaboration with the Kurchatov Institute of Atomic Energy, Moscow, our scientists took part in calculations concerning the INTOR. The equilibrium was calculated, taking into account the heat and particle losses.

The plasma-wall interaction studies comprise, on the one hand, experiments with tokamaks at the KFKI as well as at the Kurchatov Institute, and on the other hand, model experiments on surface deformation (blistering, etc.) of solid materials.

The T-10 experiments were carried out together with the scientists of the Zentralinstitut für Elektronenphysik, Berlin, GDR (ZIE). Carbon and silicon probes were exposed to the plasma of the T-10 tokamak using the surface analysis station WASA. Time resolved measurements were performed to detect different impurities and specifically deuterium deposited on or implanted in the probes in the near-wall region. The analysis has been performed by means of SIMS (in-situ) as well as by Rutherford Backscattering (RBS) and Elastic Recoil Detection (ERD) in Budapest.

The main results can be summarized as follows:

- The impurity level near the wall was very high in all phases of the discharge. In the constant current region the concentration ratio n_{imp}/n_{deut} was about 0.4 for oxygen, 0.05 for Fe-Cr-Ni and $2*10^{-3}$ for W.

- The estimated implantation energy of deuterium was about 25-40 eV in the constant current phase and higher than 100 eV during disruptions.

Another part of the plasma-surface interaction studies involved model experiments in which surface deformation of solid materials (blistering, exfoliation, flaking) was induced by bombardment with an intense beam of MeV energy helium ions.

On metallic glasses differing in composition and manufacturing technology, flaking took place at near room temperature as a result of irradiation. A layer of uniform thickness suddenly flaked off, independently of the type of metallic glasses. The surface below the flaked layer was characterized by a wave-like pattern i.e. a regular series of asymmetrical elevations *(Fig. A-6)*. Such a pattern did not appear on the annealed samples, where amorphous - polycrystalline transitions took place. Surprisingly a similar pattern was also observed on the flaked surface of single crystal silicon after 2 MeV helium irradiation. In order to explain this phenomenon, a stress model was developed.

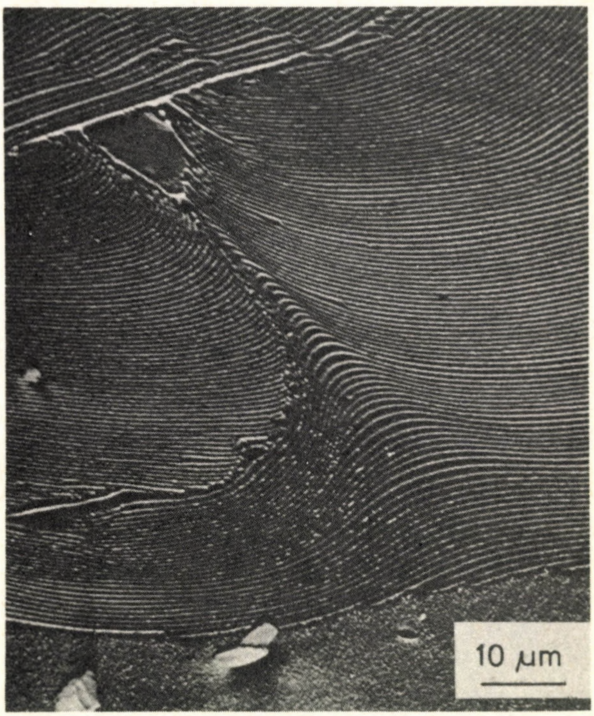


Fig. A-6

SEM micrograph of wave pattern on metallic glass after flaking

In the future fusion reactors, helium particles of a broad energy spectrum will hit the first wall. To perform quasi-simultaneous multiple energy irradiation, monoenergetic helium ions were transmitted through a periodically tilted absorber foil.

The first application of this method was the study of two competing processes, surface deformation and gas escape. Single crystal silicon covered by a 5 μm thick aluminium foil was irradiated quasi-simultaneosly by multiple energy $^4He^+$ ions up to the flux level of $3.3x10^{19}$ ions/cm^2. The implantation was performed by 3 MeV $^4He^+$ ions through a moving aluminium absorber foil. During irradiation the evaluation of the helium concentration as function of depth was measured in situ by 3 MeV proton RBS analysis. It was found that He concentration in the Al foil began to decrease after reaching a maximum value of 30 at%. This accelerated reemission process was initiated near the interboundary surface and extended inward gradually. No significant He escape was observed from the silicon during implantation, so a helium concentration of 80 at% was reached at the end of the irradiation.

The appearance of flaking clearly demonstrates that the amount of He implanted into the materials, in spite of reemission, may reach the critical value for flaking. Based on our results, the time evaluation of the implantation process and of the flaking can be described.

Fusion device first wall candidate materials were also investigated. In order to outline the energy dependence of surface deformations stainless steel and two types of inconels (EP-753 and Inco-G25) were bombarded by 0.8, 1 and 4 MeV helium beams. On EP-753 spontaneous flaking took place right after reaching a critical dose. On the other targets large exfoliations were observed without rupture. After mechanical opening of the exfoliations, a similar inner morphology was found as in our previous studies on gold.

The development of new diagnostic methods was not confined to solving merely technical problems. In some cases our scientists also obtained new physical results.

The formation and evolution of magnetic islands is of primary importance in the physics of tokamak plasmas. A direct indication of such magnetic perturbations is possible by using an energetic (150-180 keV) proton or deuteron beam as a probe which penetrates deeply into the plasma through the main confining magnetic field. A sophisticated arrangement has been constructed to perform such experiments, making use of the Cockroft-Walton accelerator NG-200 next door. The same arrangement is to be used for (in situ) measurement of the carbon deposition rate on the first wall using the nuclear reaction $^{12}C(d,p)^{13}C$.

A great part of our work was connected with laser-assisted diagnostic methods and involved laser light-plasma interaction studies.

In collaboration with the Kurchatov Institute of Atomic Energy in Moscow, a heterodyne laser interferometer was developed for the T-7 tokamak. The length of the light path in the interferometer is about 8 m long.

Twin lasers of wavelength 118 μm were developed as the light source of the interferometer. The amplifying medium, methanol vapor, was optically pumped by a frequency tunable (9-11 μm) single frequency CW CO_2 laser, designed especially for high frequency stability. The maximum power of the methanol laser is about 140 mW. The frequency stability and time dependence of the frequency of the pumping light beam was investigated (the relative stability is better than 10^{-7}).

A laser apparatus for Thomson scattering was developed and used to investigate pulsed arc discharges.

A special laser light scattering chamber was designed for use of the laser resonance fluorescence method for the investigation of laser desorption of the atomic species on the surface of the plasma chamber.

The thermal self-focusing process was studied in a laser produced plasma. The result of the process in the formation of a cavity in the plasma charge distribution and of a very intense light pencil in the light intensity distribution. Therefore the process is of importance, for instance, in the heating of the plasma with electromagnetic waves and in the compression of the pellets in laser fusion.

The laser research is going on in collaboration with the Max-Planck Institut für Quantenoptik, München, with Central Institute of Physics, Bucharest and with the Institute of General Physics, Moscow.

We are taking part in developing diagnostical equipments for the T-15 tokamak at the Kurchatov Institute for Atomic Energy, Moscow. The laser interferometer for the T-7 tokamak was a preliminary experiment for a large system on the T-15.

Other contributions will consist of some parts of a soft X-ray (1-10 keV) diagnostic system; namely gas proportional and Si(Li) spectrometers, together with their electronics, have been developed, manufactured and tested.

Complying with the requirements of our investigations, some parts of the MT-1 tokamak were reconstructed, namely the iron core of the transformer, the high current contacts of the toroidal windings and the gas inlet system. The contacts now are suitable for a current up to 140 kA instead of 100 kA, permitting up to 1.3-1.4 tesla in the centre of the toroidal field. The data acquisition system was enlarged in capacity: the computer has now a 764 Kbyte memory, more disks, more terminals, etc.

BIOPHYSICAL RESEARCH

Activity in the field of elemental analysis of biological matter has continued. In addition to the accelerator based techniques, such as particle induced X-ray emission (PIXE) and deuteron induced nuclear reactions, the radioisotope excited X-ray fluorescence method has also been increasingly applied. Interest has focused mainly on samples of agricultural origin. A fast and simple XRF method was developed for Ca, Mn, Fe, Cu, Zn and Sr content of so called premixes providing the micro element neccessities of animals in stock breeding. For investigating the mechanism of artificial fertilizing processes and improving their efficiencies fast simultaneous determination of N,K and P content of plant leaves would be desirable. The development of an accelerator based technique combining PIXE and PIGE (particle induced gamma ray emission) is in progress.

The kinetics of certain important conformational changes in biological macromolecules can be studied by time resolved flash photolysis. An optical measuring device containing a nitrogen laser driven dye-laser was built up. After careful testing, measurements will be performed to study the recombination of carbon monoxide with myoglobin after laser photolysis.

The formation of neuronal networks was studied experimentally and theoretically, as well. Nerve cells isolated from chicken embrio brain were cultured in sterile conditions. Systematic study was performed to find the optimal conditions for achieving pure neuron cultures. In order to investigate the details of network formation a special printed circuit microelectrode system is under development. With the help of this device simultaneous multi-channel electrophysiological measurements are planned.

Theoretical neurobiology offers a conceptual framework to interpret, by coherent concepts, the experimental data referring to different time and space domains, from milliseconds to decades and from Ångströms to meters. In the spirit of the mental strategy offered by dynamic system theory the development of nervous system may be particularly mentioned. The concept of "noise-induced transition" has been adopted to explain the ontogenetic formation and plastic behaviour of ordered neural structures. Deterministic and stochastic models of chemical reaction are important theoretical methods of studying dynamic biophysical phenomena.

ENGINEERING BACKGROUND

In the scientific research of this institute an important role is played by the Department of Technology. By tradition, the Department provides the engineering background needed for nuclear and particle physics research. More specifically, it designs and manufactures the highly specialized and complicated electronic instruments and devices necessary for the experiments. In the last two years the Department's activity has been dominated by the design and production of complex electronic systems and instruments for space research. The Institute's participation in the international VEGA Project is the subject of a separate article. Besides the concrete scientific instruments launched with the space probe, a firm technological foundation has been established that will serve as a base for further space research developments and also for other activities where extremely strict technological requirements have to be met. Very useful experience has been achieved e.g. in the field of component testing, quality and reliability control, assembly work in clean room etc.

In the following the main fields of the Department's activity, other than space research, will be described.

Image processing based on CCD technology has been a main field of development for several years. The first major system of this type was RIMA, which used a linear image sensor. RIMA has been used successfully in the last years for the automatic evaluation of particle tracks, making much faster the processing of the large amounts of data from high energy physics experiments. Much further experience with CCD matrices has been obtained in the VEGA programme, where this kind of image sensor is used in the TV cameras. CCD matrices will probably be widely used in the future in several scientific and industrial applications, where the results of the hardware and software development of the VEGA TV system can very well be utilised.

Much work has been done to develop and construct computer controlled measuring systems and to interface them with special peripheral devices (especially colour graphic displays). Both hardware and software has been developed by our department. The experience so obtained will be utilized in future designs.

Multiwire proportional chamber development has also been continued. For the improvement of the spectrometer of the BIS-2 measurement, carried out at JINR, Dubna, a proportional chamber with X-Y-U signal wire planes and with 2x1 m^2 active area has been designed and prepared for production.

The traditional area of development in the Department, nuclear electronics, has also been carried on. Instruments for nuclear physics experiments, especially for fusion research measurements have been built. Most of the instruments have been constructed in CAMAC. The design and the final qualification tests of an 8x256 channel pulse height analyser module have been completed. A fast phase meter module has been designed for a system measuring fast changes of the refraction index of plasma in tokamaks.

The development of a novel 16k memory module has been started. The unit will make possible simultaneous measurements with several independent nuclear ADC-s.

RELATIVISTIC HEAVY ION PHYSICS

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In the last decade relativistic heavy ion physics has developed into one of the frontier areas of physics. The possibility of studying the properties of nuclear matter at densities ρ higher than the normal nuclear density, $\rho_o = 0.15$ nucleons/fm^3, and at temperatures T higher than the binding energy of nucleons, B = 16 MeV, has opened up in the last few years. As heavy ion accelerators with higher and higher bombarding energy have been used in the experiments, larger and larger hadronic matter densities and temperatures have been reached. Presently densities of $\rho \simeq 2\text{-}3\ \rho_o$ and temperatures of T = 140 MeV (!) can be produced in a space-time volume about two orders of magnitude larger than that accessible in the particle-particle collisions. In the near future accelerators will start to operate in which a uranium beam is accelerated up to 10 GeV/nucleon energies. In this case the space-time volume will increase to about 3.000 times the space-time volume of a nucleon-nucleon collision. The temperature will be around the limiting temperature $T \approx 200$ MeV. It is very difficult to predict the maximum density, but it is estimated to be in the vicinity of $\rho \approx 10\ \rho_o$.

It is quite natural that in such a large range of densities and temperatures the hadronic matter may have many different and interesting features: such as liquid-gas phase transitions, density isomers, pion condensates, transition to the deconfined quark phase, as well as transitions to the chiral symmetric quark-gluon plasma. Especially the possibility of the phase transitions to the quark-gluon plasma attracted the interest and efforts of nuclear and particle physicists and of some astrophysicists. Here one may learn about the nature of the matter which was present at the very beginning of the Big-Bang and about the basic properties of the quantum chromodynamics, too.

The lifetime of this very hot and dense matter is short. Soon after its formation it begins to cool and expand, returning to the lower density hadronic matter. It is very important therefore to find signatures that inform us about the very hot stage and which are not destroyed during the subsequent rapid expansion. Good candidates for such messenger purposes are the strange particles. Using our hadrochemical method we have calculated the number of strange particles (K mesons, Λ and Σ particles) produced in the intermediate hadronic phase of the reaction. Then, developing a method, quarkochemistry, for calculating the number of strange-antistrange quark pairs in a dynamic quark-gluon system, the number of K mesons produced was determined. The results show that a large increase in the number of produced K mesons, and specially a very large increase in the K meson/π meson ratio will signal the formation of a quark-gluon plasma. The experimental K and π meson cross sections (up to 2.1 GeV/nucleon bombarding energy) agree excellently with the hadronic phase prediction, showing that the bombarding energy and/or the bombarding mass has to be increased to reach the quark-gluon phase [1,2].

The hot hadronic phase in itself has interesting features. In heavy ion collisions the momentum distribution of the particles may remain anisotropic even in the intermediate stage. This momentum anisotropy helps the formation of the Migdal type pion condensation, as it was shown in a relativistic mean field calculation [3]. An extended relativistic mean field calculation leads to the surprising result that above $T = 170$ MeV the effective mass of the pions will be larger than the effective mass of the nucleons [4].

During the explosion of the ball of quark-gluon plasma produced in heavy ion collisions very complicated processes are going on. Therefore, it is important to look for characteristic quantities which are conserved during the expansion phase. Such a quantity is the entropy of the system. Entropy production is increased if a rapid phase transition goes on during the heavy ion reaction [5,6]. The total entropy on the other hand is revealed in the particle composition and spectra of the reaction products. A careful analysis has shown that the measured deuteron to proton ratio is compatible with the hadronic phase and does not indicate the formation of a quark phase, as had been assumed earlier [7].

In the ultra relativistic regime, in contrast with the stopping regime discussed above, a new mechanism will dominate the heavy ion reactions. In the collision a "color rope" will be formed from the single color flux tubes. Inside of this color rope the color field is very strong. In this strong field the vacuum will be polarized, leading to quark-antiquark pair production and consecutively to pion production [8].

The measurements to be performed in the near future at the very high energy heavy ion accelerators promise to provide important, experimental tests of the present theoretical ideas.

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THE VEGA PROGRAMME

The two VEGA spacecraft were successfully launched on 15 and 21 December 1984, respectively. After reaching the planet Venus in June 1985, they are scheduled to encounter Halley's comet in March 1986.

Four space probes are to visit the comet in the same month and conduct a comprehensive study of the cometary nucleus and the coma which consists of a cloud of neutral gas, ions and dust particles. VEGA 1 and 2 will be followed by Giotto (spacecraft of the European Space Agency) and Planet A (spacecraft of Japan).

Halley's comet is a characteristic member of the family of long-period comets with a spectacular tail and coma observed many times in history. According to present understanding, the cometary nucleus is a conglomerate of dust and frozen volatile components. When the comet approaches the sun, the surface warms up causing volatiles to sublimate from a layer close to the surface. The freshly sublimated gas molecules (parent molecules) leave with a velocity near the local sound speed and drag away the dust particles. In the vicinity of the nucleus the gas density is high enough to induce chemical changes via frequent collisions and secondary (daughter) molecules start to form. At larger distances from the nucleus photodissociation of neutrals is the dominant process that gives rise to hydrogen atoms and leads to the development of a large hydrogen corona. Outflowing neutrals, ions and dust particles interact with the solar wind to produce the cometary ionosphere, dust and ion tail.

Information available at present on comets comes from remote optical observations. Direct in situ exploration of a comet promises a much deeper understanding of these primitive bodies that have preserved information on the early conditions prevailing in the presolar nebula. The principal aims of the VEGA project are: to determine the physical characteristics and chemical structure of the nucleus; to identify the parent molecules; to determine the chemical composition and size distribution of the dust grains at various distances from the nucleus; to determine the chemical composition of the coma as a function of distance; and to investigate the interaction between the solar wind and the cometary atmosphere and ionosphere.

In order to carry out these tasks the VEGA probes are equipped by an arsenal of scientific instruments completed in the cooperation of eight countries: the Soviet Union, Hungary, France, Austria, Bulgaria, Czechoslovakia, the Federal Republic of Germany and Poland. The scientific payload includes: a TV system, a three-channel spectrometer, an infrared spectrometer, a dust mass spectrometer, two types of dust impact counters, a neutral gas mass spectrometer, low energy ion-electron spectrometer, energetic particle detectors, plasma wave detectors and magnetometers. Our Institute collaborated with the Soviet Union and the FRG to develop the television system, the ion-electron spectrometer, the energetic particle telescope, the neutral gas mass spectrometer, the pointing system of the platform and the data acquisition system.

The TV system is designed to fulfill a complex scientific and technical task: automatic recognition of the comet and its nucleus; tracking of preselected regions; imaging of the comet with high angular resolution in various spectral ranges; and transmission of the images to the Earth. From a distance of 10^4 km, the narrow angle camera should achieve a 100 m resolution to form an image of the nucleus, something that has not yet been done due to the optically thick coma. Main scientific objectives are to obtain pictures of the nucleus to determine its size, its shape, some surface and photometric properties, the existence of jets, the rotation period and the spin axis as well as to observe the tail near perihelion. The two VEGA are also planned to provide Giotto with more accurate orbital information on the comet to help it in reaching an 500 km approach from the nucleus.

The ion mass spectrometer and electron analyzer consists of three sensors; an ion spectrometer oriented parallel to relative velocity vector covering the energy range of 15 eV - 25 keV. If the thermal velocity of cometary ions is much lower than the encounter velocity a mass spectrum in the range of 1-100 amu can be obtained. Oriented towards the Sun, a second ion sensor will detect particles of energies between 50 eV and 25 keV. A single-channel electron analyzer will measure electrons in the energy range of 3-3500 eV. Questions to be answered by the experiment include: how do the solar wind parameters change during the approach; is there an inner shock and what is its location; how do plasma parameters change across the shock front; what is the location of the ionosphere boundary; and what is the chemical composition of ions in the ionosphere, as well as outside the bow shock.

The energetic particle telescopes (TÜNDE-M) are to detect ions accelerated in the vicinity of the comet, to measure their energy (in the range of 20 to 640 keV), flux and angular distribution (by two independent telescopes with different orientations). The detectors extend the ion measurements to those accelerated by the solar wind, i.e. to larger energies or larger masses. The continuous operation of both charged particle detectors throughout the 15 month voyage to the rendezvous with the comet will allow the collection of reliable data on the ion background as a function of solar activity and, in addition, will permit the observation of solar particle events that occur during this period.

Two flight models and a spare model of the TV system, the data acquisition system, energetic particle detectors and the ion-electron mass spectrometer were completed in the institute, together with the earth based control unit for the neutral gas analyser.

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RESEARCH INSTITUTE FOR SOLID STATE PHYSICS (SzFKI)

This Institute deals mainly with basic research. Recently, however, in addition to traditional optical and solid state physics, our research activities have been broadened and now include some research-and-development R&D topics mainly along the national research direction "Solid state research".

Research is in four main areas:

1. lasers and spectroscopy
2. theoretical solid state physics
3. research on metal physics
4. partially ordered condensed matter research.

Examples of our "D" activities are laser systems for industrial and/or medical applications, technology of metallic glass production and their different applications, which are discussed briefly under their corresponding area headings. The list above does not contain the engineering work of applied electronics and equipment design, or dynamic neutron radiography for industrial testing. Examples of this engineering work are described separately.

This progress report contains summaries of the four main subjects, each supplemented by a corresponding list of references, following, as it is now a tradition, by brief surveys of selected research-and-development topics submitted for the 1985 "Jánossy Award" of the Central Research Institute for Physics.

DEVELOPMENT AND RESEARCH OF LASERS

In the course of basic research connected to lasers we succeeded in showing experimentally the existence of an effect predicted long ago by theory, namely the induced optical tunnel-electron emission from noble gas atoms and metals. In the experiment a 10.6 μ infrared wavelength CO_2 laserbeam was applied. A new result of the "Halo" laser, which radiates light in every direction of a plane, is the discovery of the previously unknown two dimensional "chaterine"-modes. It was possible to describe the features of these modes by a simple model.

An effect discovered in 1980, the reorientation of nematic liquid crystal layers by the electric field of a laser beam was studied further with more sensitivity in the special case of total internal reflection. We succeeded in building an apparatus in which even at low light intensities (1 mW, $40W/cm^2$) the liquid crystal changes from the totally reflecting state to the transmitting state. In this way it was possible to construct light controlled optical switches.

Experiments were carried out on Al-oxide-Ag and Al-oxide-Au type thin film tunnel diodes using an Ar ion laser to investigate internal photoelectric effect. It was found in the case of a grating substrate that the photon-electron yield is maximum if the momentum conservation law is also satisfied for the top metal-vacuum surface plasmons. The values for the surface plasmon dispersion relation and the overall quantum efficiency were the same as those obtained from internal photoelectric effect and light emission measurements. This agreement verifies the reversibility of the processes.

In the investigations performed on hollow cathode gas discharges by using a discharge tube of a special geometry an anomaly was observed in the voltage-current characteristics at low He and Ne pressures. The anomaly could be explained by the transition of the hollow cathode discharge to a plane cathode type discharge. A special tube processing technology was developed in the course of work on the hollow cathode He-Kr laser, and using this a d.c. excited laser, radiating 12 mW output power at the 469.4 nm transition of the Kr ion, was built. It further was found that the optimum gas pressure and the optimum mixture ratio depend strongly on the value of discharge current.

The prototype of a miniature water-cooled Nd-phosphate-glass laser operating at a repetition rate 1Hz was completed, and the laser is now ready for serial production. Its parameters in Q switched mode are: pulse length 15 nsec and radiated energy 7 mjoule, and in the free generation mode 150 μsec and 1 joule, respectively. Experiments were started to find applications of this laser in science, industry, biology and medical treatment.

In work connected to development of the YAG laser, the coupling of a low loss optical quartz fiber to our MEDI-YAG medical apparatuses was accomplished for use in gastroenterology, urology, pulmonary examination and gynaecology.

An interferometric measuring system using a laser was developed for the measurement of different geometrical parameters (linearity, velocity, distance, angle and straightness). Using a frequency stabilised He-Ne laser as a light source, the intelligent evaluation system is particularly suitable for quality control in the machine industry and for machine measuring tasks.

Our thin film evaporating laboratory produced a large number of various interference filters and laser mirrors for internal and external (Hungarian Optical Works, Labor MIM) use.

SOLID STATE THEORY RESEARCH

Considerable progress has been made in the study of the physics of phase transitions. The nature of the first order transition and the non-universal behaviour was studied in a Hamiltonian version of several spin models. The ground state properties of $S \geq 1/2$ antiferromagnetic Heisenberg chains were also studied by numerical methods. Furthermore, we examined the low energy excited states in a Hubbard chain with on-site attraction. In spin glasses the low temperature relaxation and the spin-spin correlation have been studied by using statistical physical methods. We have developed a model description for the ferroelectric phase transition. The multicritical behaviour has been described below the antiferrodistortive transition in $LaAlO_3$.

We studied the properties of a fully developed chaos in one dimensional maps. The calculation of entropy was also discussed in chaotic systems.

In the field of metal physics we continued our study of the interaction between electrons and 2-level systems in amorphous metals. We calculated the electronic structure and examined the alloy formation processes in alkali-gold compounds. The properties of ferromagnetic transition metals were investigated at finite temperatures. In the study of granular superconductors, it has been recognized that in the paraconducting state phase coherence reaches its maximum at finite temperatures. This gives a clue to understanding the resistance minima in granular samples. The nature of the low-temperature phase coherence of valence fluctuations has been described by using a variational ground state wave function.

We derived a one dimensional microscopic quantum theory to describe the interaction of a single impurity with a charge density wave (CDW) at zero temperature. The following physical quantities were calculated: electron density, ground state energy, density of states, the force exerted by the impurity on the CDW as a function of the impurity position relative to the CDW. A solution for the equation of motion was also found.

The Bose-condensed phases of spin polarized atomic hydrogen were described using a quantum mechanical S = 1 spin model. We examined the activated tunneling decay of metastable states. In the field of electron localization we studied the effect of localization on impurity dynamics in the case of a Kondo impurity and for two-level systems. The electron localization in disordered systems and the metal-insulator transition was also studied.

We have continued to study the interaction of electrons with strong electromagnetic fields (laser). The properties of Rydberg-atoms in weak magnetic fields and the wave propagation in non-linear waveguides were also examined.

RESEARCH INTO THE PHYSICS OF METALS

Research in metal physics concentrated on amorphous metals involved a broad variety of projects ranging from the study of the problems of rapid solidification, through the detailed investigation of the structure and the physical properties, and ending with the search for practical applications of the metallic glasses.

A great number of metal-metalloid and metal-metal type amorphous alloys have been prepared by rapid solidification techniques.

A theoretical model has been developed for the continuous casting of metallic glass ribbons on the basis of an infinite viscosity assumption. A new production method, the splat cooling, has been installed in the metallurgical laboratory. This method, working in inert gas atmosphere, yields 10-15 μm thick amorphous samples.

We continued the investigation of the thermal stability of amorphous metals by calorimetry (DSC). Mössbauer spectroscopy, neutron diffraction and small angle neutron scattering measurements were also performed on transition metal-metalloid and metal-metal type glasses.

In accord with earlier results, we found that in transition metal-metalloid glasses there are well defined atomic environments and they can be described in terms of the local atomic order that exists in the corresponding crystalline phases. A very good example was given by a high resolution time-of-flight neutron diffraction measurement performed on a Fe-B and nickel rich (Fe,Ni)-B glasses. The pair correlation functions show significant difference between the first neighbour environments of the glasses, reflecting the chemical difference between iron and nickel.

In the frame of a cooperation with the Turku University (Finland) an energy dispersive X-ray diffraction method (EDXD) has been developed to study the rate of crystallization, as well as the crystalline phases, themselves, during the crystallization of metallic glasses. The performance of the method was demonstrated in a study of the crystallization of Fe-P and Fe-B glasses.

Study of transport properties of ternary ferromagnetic amorphous ribbons, based on an $Fe_{80}B_{20}$ alloy was carried out. The concentration and type of the third transition metal additives were systematically varied (3d, 4d and 5d type metals). It was found that the shift of the low temperature resistivity minimum strongly depends on the magnetic characteristic of the addition metal. The experimental data were processed with a fully automatic data collecting system based on a KEITHLEY 181 DnVM and on a NEZ-215 personal computer.

In collaboration with the Csepel Non-Ferrous Metal Factory of Csepel Works we have investigated the effect of the process conditions on the physical (mainly magnetic) properties of rapidly quenched $Fe_{40}Ni_{40}B_{13}Si_7$

metallic glass ribbons. The correlations among the process parameters and the physical properties were determined using a modified version of BMDP9R ("All possible subset regressions") program.

In this investigation about 100 samples were prepared from about 10 kg of alloy. The results have shown that an empirical cooling rate proportional to the thermal conductivity of the chill block and to the inverse ribbon thickness plays a dominant role in determining the ribbon characteristics.

Investigation of the magnetic aftereffect was begun on a metallic glass with composition of $Fe_{4,5}Co_{69}Cr_4B_{20}Si_{2,5}$. A qualitative interpretation of the observed anomalously large accomodation and disaccomodation of the permeability was worked out.

Structural relaxation of an Fe-Ni-B metallic glass with low Curie temperature was investigated by means of Curie point measurements. We succeded in separating the irreversible and reversible parts of structural relaxation, and we obtained two distinct activation energies in the reversible relaxation.

In addition to the rapid quenching techniques, electrodeposition and chemical reduction have been used for the preparation of amorphous alloys (nickel-phosphorous and nickel-transition-metal-phosphorous alloys).

In cooperation with Csepel Iron Works we achieved significant improvements in these methods. A wide range of experimental techniques have established the increased quality of the newer samples in macroscopical and microscopical inhomogeneity compared to those produced by earlier preparation methods. Thus we have the capacity to produce better quality samples for basic and applied research. The electric transport features, as well as magnetic properties, crystallization processes and nuclear magnetic resonance (NMR) parameters of the prepared samples were investigated. On the basis of these examinations the macro- and microinhomogeneities, electron structure-fluctuation, conductivity and magnetic properties of the Ni-P metallic glasses were quantitatively characterized over a wide concentration range. The short range order of metalloid atoms were studied as well. We were the first laboratory to apply solid-state high resolution NMR methods, for the investigation of metallic glasses.

Specific actions that have resulted from our program are:

a) We applied for a patent for producing disconnectable electrical contacts. At present experimental production is in progress in the Telephon Factory (Telefongyár);

b) We obtained a patent for producing a nearly temperature independent electronic resistor. Experimental production is arranged with the company REMIX;

c) In the Csepel Iron Works extended investigations are being carried out for the application of corrosion and wear resistent metallic glass coatings.

PARTIALLY ORDERED CONDENSED MATTER RESEARCH

Partially ordered systems continue to be an important area of solid state research.

The non-additive behaviour of liquid crystal binary mixtures has been investigated by X-ray, thermal, spectroscopic and dielectric methods. The dipole-dipole interaction and the coupling between soft and rigid molecular segments proved to be the main factors in generating induced smectic phases.

The thermomechanical effect and its dependence on the cell thickness has been studied in cholesterics in order to determine the coupling coefficient.

Investigation of ferroelectric smectics of chiral structure has been initiated. Homologous series have been synthesized and the alignment of samples of different thicknesses has been determined. Textures and phase diagrams have been studied with a polarizing microscope. Spontaneous polarization, switching time and the Goldstone and soft dielectric modes have been measured.

Structural and dynamical properties of fast-cooled liquid crystals have been studied by means of neutron diffraction, small angle neutron scattering, calorimetry and Raman spectroscopy. The phase diagrams of the solid modifications of MBBA and EBBA have been established. We described multi--mode polymorphism and characterized the structure of some mesophases as well as the relaxation of the glassy state.

The local order in the $Fe_{100-x}B_x$(x=14, 19, 25 at%) metallic glass was investigated by high resolution neutron diffraction and small angle neutron scattering. Small inhomogeneities were observed in the samples of the off-stoichiometric compositions, which were identified as iron rich clusters. The structural parameters characterizing the short range order were determined, i.e. the partial first neighbour distances, the width of their distribution and the coordination numbers. The experimental results were interpreted on the basis of the quasi-crystalline model calculation.

Measurements were carried out with the three axis spectrometer to study two-magnon bound states predicted by theory. The existence of such states were indicated by experiments on antiferromagnetic $FeCl_2$ single crystal at low temperatures.

The dynamics of pig immunoglobulin-G (IgG) in deuterium oxide solution was investigated by the neutron spin echo technique. It was possible by this technique to study intramolecular motion without introducing probes in the macromolecule. The effective diffusion coefficient was obtained as a function of the transferred momentum. The data were interpreted as reflecting a relative wobbling type motion of the three parts of the IgG molecule.

In cooperation with the Leon Brillouin Laboratory at Saclay, an extra high resolution neutron spin echo spectrometer is being constructed, which will begin operation in 1985. A high-transmission, disc type neutron velocity selector operating in a wide wavelength range was designed and built for this spectrometer.

The Ge-Se family of chalcogenide glasses was studied. This system is ideally suited for examining effects of changes in chemical composition, of preperation conditions and of energy exchange with the environment. Amorphous Ge_xSe_{1-x} thin films and bulk glasses were prepared under various conditions (oblique deposition, slow and fast cooling, annealing at different temperature etc). Photoluminescence and positron annihilation measurements were used to map the defect structures while far-IR spectra were taken to obtain information on the structure. On the basis of our findings a new model was proposed which emphasizes a distribution of glassing temperature values in clusters or microregions of amorphous materials.

The hydrogenated silicon technology based on the glow discharge deposition method was further developed. It was proposed to use doped amorphous silicon of n and p type to form p-i-n junctions. These should have higher efficiency as solar cells than the simple p-n or Schottky type cells, and they would have the additional advantage of keeping the cheapness of the amorphous silicon technology.

Systematic investigations were begun on electrical and photoelectrical properties of amorphous silicon and their dependence on the structure and morphology of the layer. The scanning electron microscope, IR and TEM studies show that the morphology of the amorphous silicon layer is highly determined by the substrate temperature and by the RF power and also by the gas mixture itself. Layers of poor homogeneity have very poor electrical and photoelectrical properties and poor photovoltaic efficiency. Layers of good homogeneity show better transport properties and better efficiency. The mobility of the charge carriers and efficiency are near those of amorphous silicon layers reported in the literature. We have developed a simple and efficient method to characterize the photoelectrical properties of a-Si solar cells.

Transport and electrochemical properties of doped and undoped polyacetylene were investigated.
The structure of mechanically stretched, deuterated trans polyacetylene was studied by neutron diffraction. Studies on quasi-one dimensional conductors are described in another section of this Yearbook.

ELECTRON-PHOTON INTERACTION IN MOM STRUCTURES

Zs. Szentirmay

It was shown previously that fast electron irradiation of a metal-insulator interface excites plasma waves and gives rise to photon emission [1]. There is, however, a cheaper method to do this. In this method planar thin film or point contact tunnel structures are used, with low energy (2-4 eV) electrons being injected from a DC battery into the metal film.

Since an energy of a few eV is sufficient to generate surface plasmons (SPO) and photons in the visible range these structures can be used as light sources. Inversely, surface plasmons excited with light emit electrons into the barrier (internal photoeffect). Consequently, the same structure can work as light detector, too. Their extremely small size and low cost predestine these metal-oxide-metal (MOM) structures for practical applications in the microelectronics and integrated optics. However, the overall quantum efficiency of the plasmon mediated electron $\leftrightarrow$ photon interaction is very low (10^{-9}-10^{-4}), which still prevents practical utilization of MOM diodes.

As early as 1969, experimental evidence was found that tunneling electrons excite the top layer surface plasmons in a metal-semiconductor diode [2]. Nevertheless, the first light emitting MOM diodes were constructed only much later (in 1976) [3].

In these and subsequent studies it was assumed that electrons tunnel inelastically and excite a special, long wave-vector surface plasmon mode in the barrier region. This soft SPO mode (the junction mode) emits photons only via scattering on surface roughness with periods 10-100 Å. Most of theoretical works explaining electron-photon interaction in MOM structures are based on this simple model [4]. Latest experimental results, however, indicate that the light generation process cannot be explained exclusively by such a simple model and that the real electron-photon transition is much more complex [5].

Our experimental activity has been motivated by the hope that the understanding of the fundamental processes may lead to fabrication of MOM tunnel diodes of practical importance.

The experiments were performed on Al-Al_2O_3-M planar diodes where M=Ag,Au and Cu. They were prepared by thermal evaporation in $\sim 4\cdot 10^{-4}$ Pa vacuum on smooth and periodically corrugated (holographic grating) glass and sapphire substrates. A 1 mm wide, 50 nm thick Al film was first evaporated at a rate of 0.8-1 nm/s onto the 18x18x0.5 mm^3 substrate. The surface of this stripe was oxidized in dry oxygen of 4-6 Pa pressure in the plasma of a 2 kV DC discharge. Four 1 mm wide films of M, perpendicular to the Al stripe were then evaporated up to 20-35 nm thickness, forming simultaneously four 1 mm x 1 mm Al-Al_2O_3-M diodes on the substrate. The resistivity of these diodes was measured in a four terminal connection arrangement by means of a current generator technique. The thickness of the oxide layer as calculated from the zero bias resistivity was typically $d \sim 2.5$ nm ($R_o \sim 60\ \Omega/cm^2$). The periodically corrugated surface of the substrate was prepared by the standard holographic technique, i.e. a photoresist film was exposed by a He-Cd or Ar-ion laser and etched by freon gas after development. Scanning electron microscopic studies showed that the periodic grooves have trapezoidal profile. The lattice parameter a of the grating was determined from the angle of the diffracted light of a He-Ne laser while the depth of the grooves, h could be calculated from the intensity of the diffracted light. Gratings with a=302-845 nm and h=6-55 nm were used. Angular and spectral distributions of the light emitted from the diodes biased with 2-4 V DC voltage were measured between 80 and 300 K with a high sensitivity spectrometer equipped with a cold finger type liquid nitrogen optical cryostat. Typical spectra of photons emitted from an Al-Ox-Ag diode are shown on *Fig. B-1* in terms of the bias. Estimated quantum efficiencies were 10^{-7}-10^{-8} and 10^{-5}-10^{-4} photon/electron for smooth and grating substrates, respectively.

Intensity of the emitted light was found to be a logarithmic function of the thickness of top (anode) layer. Its increment is correlated with the mean free path of tunneling hot electrons in the anode metal. It was therefore concluded that these tunneling hot electrons may directly emit light when they interact with the potential jump on the top metal-vacuum interface [6].

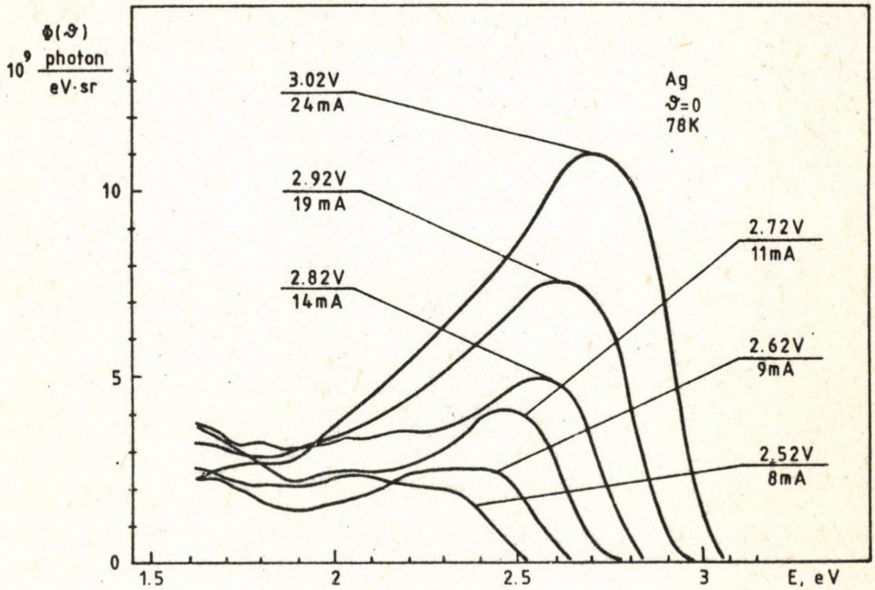

Fig. B-1

Spectral distribution of photons emitted by a MOM diode with Ag anode. Smooth glass substrate

Angular dependence measurements on grating substrates were used to determine the dispersion relation of radiation. These experiments prove that large part of the emitted light originates from the top metal-vacuum surface plasma oscillations and not from junction plasmons as predicted by several theories [7].

The strong correlation between surface plasmons and the angular distribution of emitted light permitted the study of the optical constants of gold above the 3d-band edge (2.5 eV) [8].

For deep gratings ($h > 0.01a$) a unique dispersion anomaly was discovered. At the intersection of the $n=+1$ and $n=-1$ dispersion branches a momentum gap was observed, the magnitude of which proved to be proportional to the depth of grooves (*Fig. B-2*). Analogous to the way in which light propagates in or above a medium with distributed feedback, plasma waves can interact on the grating surface when the Bragg condition is satisfied [7].

In internal photoeffect experiments MOM diodes were illuminated with the light from an Ar^+ laser and the induced current was measured in terms of the angle of incidence. Surface plasmon resonances were observed at the same angles as in the emission experiments. The quantum efficiency of internal photoeffect was measured to be of the order 10^{-5} electron/ photon, i.e. about the same as in the direct electron → plasmon → photon case. This leads to the conclusion that in the electron ⇄ SPO ⇄ photon chain the bottleneck is the electron ⇄ plasmon excitation process having the smallest efficiency. This process determines therefore the probability of the electron ⇄ photon conversion [9].

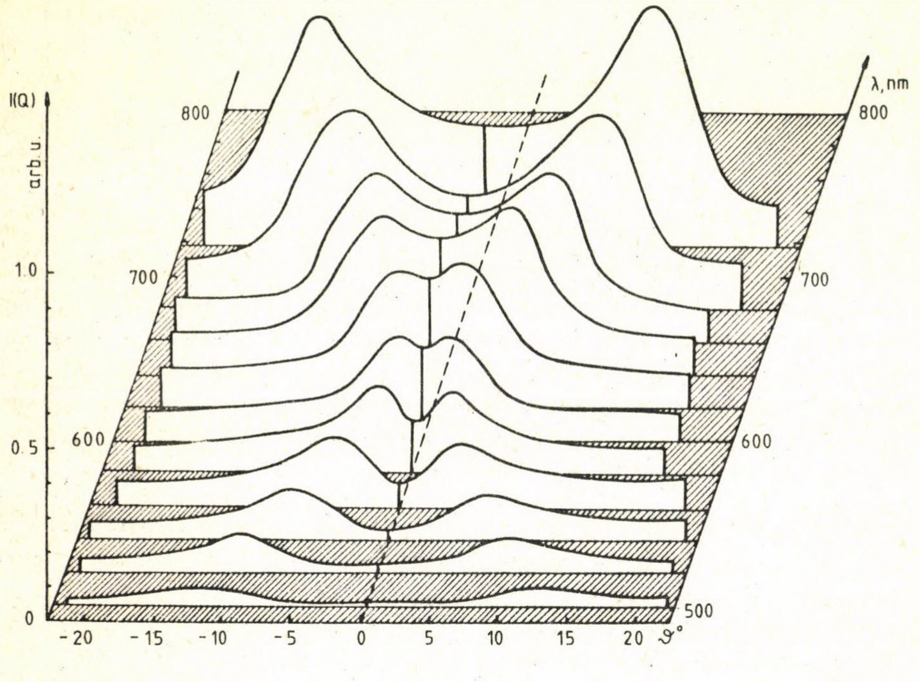

Fig. B-2

Angular dependence of light emitted by an Al-AlOx-Ag diode at different wavelengths λ. a=555 nm, h~52 nm, T=-105 °C and U=+2.5V

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THEORETICAL STUDY OF THE INTERACTION OF INTENSE RADIATION WITH MATTER

J. Bergou, S. Varró

In connection with the recent development of high power lasers considerable experimental and theoretical effort has been devoted to the study of fundamental processes in the presence of a radiation field. Our research has concentrated in two main areas. One is the exploration of the possibility of high resolution spectroscopy based on nonlinear optical methods. Equally important, however, is the study of modifications introduced by an intense radiation field into elementary processes of single charged particles. This study can lead to better insight into the microscopic nature of electromagnetic interaction. Although our activity extends to both of these fields, the greater emphasis is on the second.

Earlier, we have worked out a perturbation method for the description of intense field processes which uses the exact quantum mechanical states of an electron in a radiation field (Volkov states) as in and out states of scattering processes (see Yearbook 1981-82). In the present period we extended our method to the case where, in addition to the radiation field, an external magnetic field also participates in the process under study. In particular, we obtained the exact solution of the corresponding Dirac and Klein-Gordon equations and determined the cross section for potential scattering of relativistic electrons in the simultaneous presence of a laser and a magnetic field. Since this is just the elementary process in induced bremsstrahlung, we could predict a resonance structure of the scattering arising from laser induced transitions between Landau levels caused by the magnetic field.

One of the problems in the scattering of electrons in the simultaneous presence of a strong radiation field and a magnetic field is the fact that in the zero magnetic field limit one does not recover the formulae derived in the magnetic-field-free case as long as one considers the transitions to occur between Landau states during the scattering process. The source of this inconsistency is the application of Landau states which do not reproduce free electronic states in the zero magnetic field limit. In order to solve this problem we have constructed coherent states of the electron in the magnetic field and we have proved that a special class of packets of coherent states is able to reproduce free electron states in the appropriate limit. The coherent states of an electron embedded simultaneously in a radiation field and a magnetic field have also been constructed and applied in a semiclassical description of the magneto-Raman scattering of laser light in the presence of a nearly resonant strong microwave (the frequency of the microwave was assumed to be close to the cyclotron frequency). This latter process is of some practical importance for laser diagnostics of a magnetized plasma where the microwave adds new features and enhancements to the predicted scattering spectra. We have also carried out the exact fully quantum-mechanical analysis of the scattering of high frequency laser radiation by electrons in the presence of a strong magnetic field and an intense microwave field.

Our investigations in the above fields naturally led to the study of a general problem: the question of gauge invariance of the quantum mechanical description of optical transitions. We managed to show that the commonly used forms of the interaction Hamiltonian all lead to the same gauge-independent results provided that there is an appropriate switching on and off process of the interaction. Furthermore, the system has to be prepared before the interaction is switched on and its final state is observed after the interaction is switched off. This condition is fulfilled in most experiments. If observation is carried out while the interaction is on special care must be taken in order to satisfy the requirement of gauge-invariance of a theoretical description.

We have also dealt with an exciting problem of atomic physics. Recent experiments on Rydberg atoms in a magnetic field led to the conjecture of a "hidden" symmetry. The problem of theoretical description is twofold: the quadratic Zeeman term leads to a nonseparable Hamiltonian and the large principal quantum numbers involved in the experiments ($n \sim 30$) lead to a highly degenerate case (degeneracy $\sim n^2 \sim 1000$). Therefore, the usual perturbation methods are inapplicable. We succeeded in developing a new method, based on the classical aspects of the problem, that is capable of describing the observed phenomena. With its help we have predicted some new effects which will occur if, in addition to the magnetic field, an electric field is also applied. Specifically, because of the breaking of the reflection symmetry in a magnetic field, part of the spectrum exhibits a linear Stark shift and the rest exhibits a quadratic one.

Finally, we investigated some nonlinear optical phenomena which, besides their principal interest, may find an application in integrated optics. We studied reflection and refraction from the surface of a nonlinear material, mainly in the domain of total reflection. With the help of these results we obtained the mode structure of a slab waveguide in which the slab is linear and the surrounding is nonlinear. The mode structure becomes intensity dependent and in a certain range of intensity soliton type propagation may occur. Furthermore, the switching from usual to soliton type guidance occurs in jumps with hysteresis, i.e. the system exhibits bistability. The most interesting aspect of the problem is, however, symmetry breaking. In a symmetric structure one can find eigenmodes where the intensity distribution is asymmetric. The system is easily accessible and thus, besides immediate applications, it is extremely well suited to the study of such fundamental phenomena as phase transition--like processes in nonlinear systems.

SEARCH FOR THE APPLICATION OF METALLIC GLASSES

A. Lovas, J. Szöllősi, J. Takács, L.F. Varga

A search for the application of metallic glasses has begun in the Institute. The efforts are concentrated on the use of metallic glasses as soft magnetic materials, resistors and fibre reinforcement.

Fe-Si-B-C amorphous ribbons have been used as a noise suppressing choke in electronic and high power circuits. In *Fig. B-3.* the scheme of a dc power supply is shown. The former ferrite cores have been replaced by metallic glass ones. These devices are very cheap and easy to produce.

Figure B-4 shows a transformer containing two specially wounded amorphous ribbon cores (patent pending). The high permeability metallic glass ribbon has much better frequency characteristics than the usual permalloy core. This VLS T40 transformer has been designed as a step-up device for very low audio frequency signals especially for use with moving coil pick-up cartridges. The transformer will increase by a factor of 30 the input voltage of a high fidelity amplifier without distortion. It consequently ensures high quality sound reproduction and a high signal-to-noise ratio at high output power of the amplifier.

The metallic glasses can be used as special resistivity materials. This notion is based on the high specific resistivity of the rapidly quenched non-crystalline alloys. In addition to the high resistivity a very low (less than 10 ppm/K) temperature coefficient can be attained with some nickel-chromium based metallic glasses (patent pending).

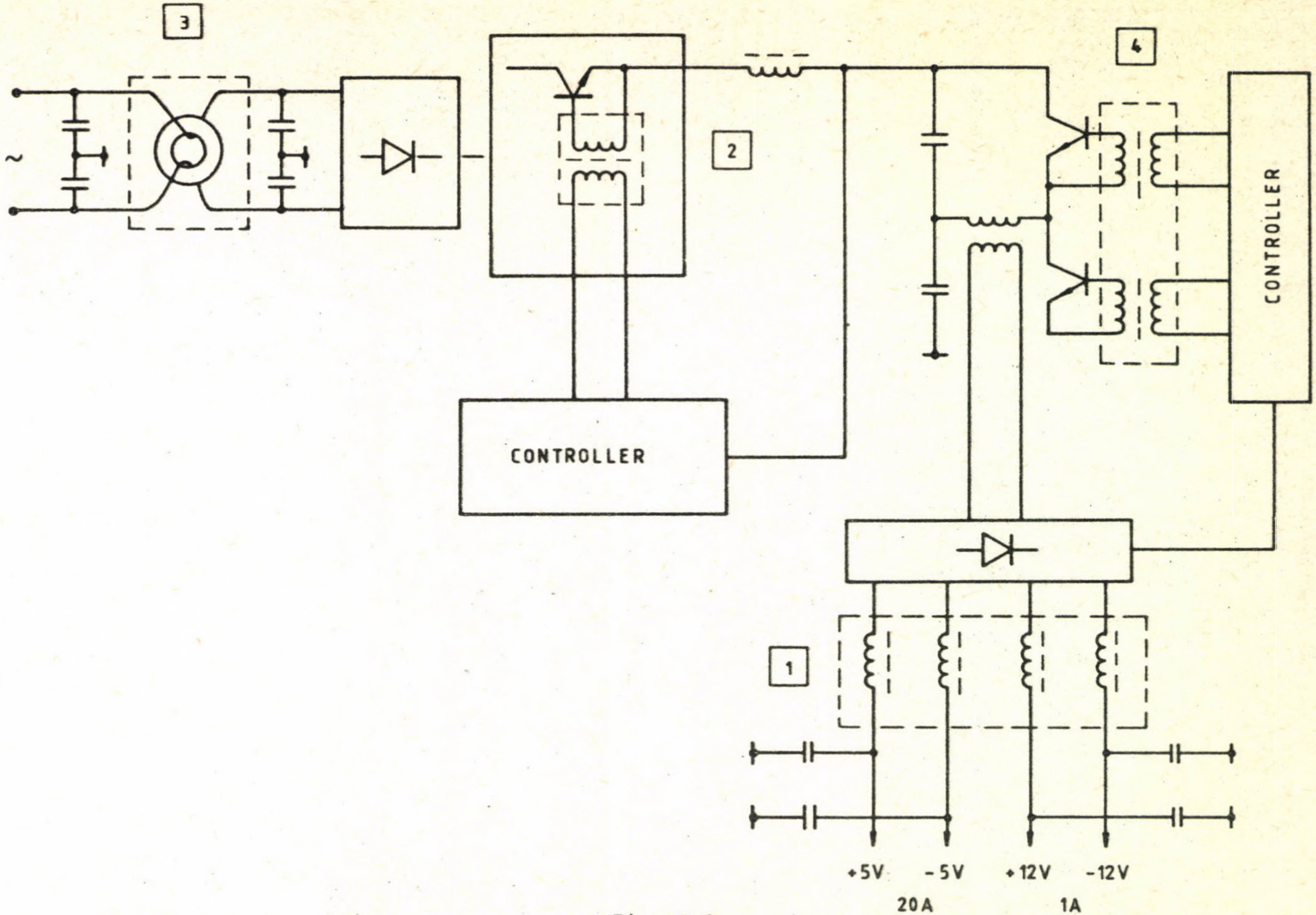

Fig. B-3

The scheme of a dc power supply. The driver transformers and line filters in dotted frames are made of amorphous ribbons.

Fig. B-4.
VLS-T40 amorphous alloy transformer

Recently, fine ribbons of a metallic glass, developed in cooperation with company DUTÉP, have been succesfully used as fibre reinforcement in concrets.

CHARGE DENSITY WAVE DYNAMICS IN QUASI ONE DIMENSIONAL SOLIDS

Gy. Hutiray, A. Jánossy, K. Kamarás, Gy. Kriza, Gy. Mihály and L. Mihály

A great number of strongly anisotropic organic and inorganic systems undergo a metal - insulator transition related to the instability of a quasi one dimensional electron system against perturbations with a wavevector $q=2k_F$, where k_F is this Fermi momentum. Below this so-called Peierls transition the electronic density is oscillatory in space and is coupled to a similarly oscillatory lattice distortion. In several cases this "charge density wave" (CDW) is incommensurate with the underlying lattice and its phase is determined by a weak coupling to impurities. In some high purity compounds small electric fields may overcome this weak restoring force and a collective current carrying mode of the coupled electron-phonon system occurs.

We have performed a detailed study of the transport properties of orthorhombic tantalum trisulfide (o-TaS_3), a prototype of materials in which this collective mode, the so called sliding charge density wave conductivity, has been observed. High purity fibrous single crystals were grown in our laboratory. Various experimental methods were used to determine non-linear current-voltage characteristics, frequency dependent conductivity and dielectric constant and thermoelectric power. We have shown that in o-TaS_3 metastable states can be created by thermal treatment. These metastable states are indicated by a change in the normal conductivity. Once the system is brought out of equilibrium the metastable states decay logarithmically as a function of time in a manner somewhat analogous to the magnetization of spin glasses. We have established a simple model to describe this relaxation. Small electric fields rearrange the metastable charge density wave states. The experiments also show that a sliding CDW current gives rise to a deformation of the CDW: after the current is switched off the system is found in an inhomogeneous metastable state in which the normal resistivity depends on the position. We have suggested that a number of electric and thermal memory (or hysteretic) effects may be understood by a simple model of deformable CDW-s. We assume that metastability is related to a non-equilibrium charge transfer to the metal chains giving rise to a slightly inhomogeneous wavevector.

We have investigated the role of impurities in the sliding CDW mode. Defect concentrations of the order of 10^{-6} per Ta atoms affect greatly the pinning force acting on the CDW, as seen by a dramatic increase of the threshold electric field required for its depinning and the decrease of the low frequency dielectric constant.

We found that, to a good approximation, the sliding charge density wave mode carries no heat, or at least very little heat compared to normal electrons.

NEUTRON RADIOGRAPHY

M. Balaskó, L. Cser, F. Deák, L. Róth and E. Sváb

All over the world interest is increasing in non-destructive material testing. With the help of these methods the structure or composition of an object, or the result of a technological process can be tested without damaging the object or making it unsuitable for further use. Neutron radiography is an advanced technique for non-destructive testing by transparency. In principle it is similar to X-ray or γ-radiography. However, the peculiar transmission properties of neutrons provide results which are complementary to classical radiography or may provide completely original information.

Neutrons are transmitted by the majority of the technically important metals (e.g. aluminium, iron, steel, copper) with little loss. However hydrogen-containing materials, like water, oil or several types of synthetic compounds cause a significant decrease in the intensity of neutron radiation. These special transmission properties enable neutrons to be used for obtaining information on the inner structure of objects or to investigate hydrogen-containing fluids in metal tubes.

Several neutron radiography laboratories connected with research reactors have been built in Europe. In them photographic methods are used, enabling only static images to be made. Dynamic neutron radiography, suitable to record movements within the objects has only been realized in Great Britain (Harwell).

We have been successful in producing an arrangement suitable for static and dynamic neutron radiography tests. This will allow us to introduce these testing methods in Hungarian industry as well as to do research for the further elaboration of the method.

SOME CHARACTERISTICS OF OUR NEUTRON RADIOGRAPHY INSTALLATION

A high efficiency dynamic neutron radiography system (*Fig. B-5*) has been developed at the WWRS-M type 4.6 MW research reactor using thermal neutrons of about 10^8 n/cm^{2}s flux at the object position. A scintillation

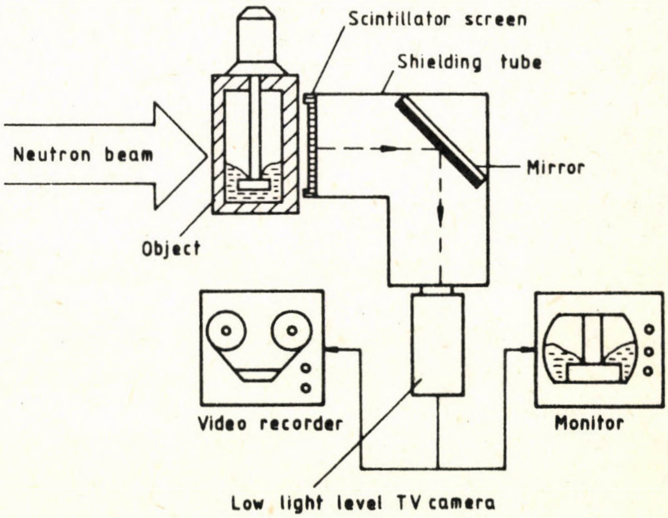

Fig. B-5.
Dynamic neutron radiography experimental installation

screen and a low light level camera are used to detect the neutron radiography image of the investigated object. The light obtained from the neutron screen is turned by 90° by a mirror in order to avoid activation damage to the camera caused by the beam. The imaging cycle of the camera is 40 msec providing thereby the possibility for visualizing medium speed motions. In addition to the neutron radiography image some physical parameters (e.g. temperature, measuring time, pressure) of the investigated object may be visualized on the monitor and recorded on the same video tape for further evaluation.

No γ-ray filter has been placed into the channel, so the reactor can be used as γ-ray source, too. In this way, gamma- and neutron radiography can be applied simultaneously, which is very advantageous in several cases.

After a number of demonstrations, industrial contacts were made in several fields. The most important are the following:

INVESTIGATION OF ABSORPTION TYPE REFRIGERATORS

The working fluid of absorption type refrigerators is a mixture of water and ammonia. The high hydrogen content of this fluid enables to visualize the processes of boiling and transfer in the bubble pump within the double-walled pipe. The condensation of ammonia gas in the condensator, the formation of drops in the evaporation system and the level of fluid in the tank can be measured with high accuracy. Any inaccuracy in the relative position of the coaxial tubes and dirty spots in the system become clearly visible. Neutron radiography investigations gives a possibility of optimalizing power and of increasing efficiency.

STUDY OF INNER PROCESSES OF A HEAT PIPE

The heat pipe is an increasingly popular device of present day heating technology. With the help of our method, the circulation of the working fluid (e.g. water, natrium) such as boiling, condensation and leading back of the condensate may be visualized. In the case of gravitational heat pipes we have tested our technique under industrial circumstances. It was observed that the great volume of gas bubbles created during boiling causes pulsing flow of the fluid which, in turn, causes a periodic drying of the inner surface of the heated pipe. This phenomenon has not been described in the literature and will be a very important consideration for engineers planning heat pipes.

VISUALIZATION OF INTEGRATED CIRCUITS

Radiography enables the testing of electronic devices. It was used for controlling the placement and connection of components embedded in plastic (condensors, resistors, transistors etc). Neutron radiography was complemented by gamma radiography -using the reactor as gamma source- and so we have a complete picture of the metal and plastic components.

Some further applications: the circulation pump system of a stream cromatograph has been tested; the streamline picture of fluids circulating in metal pipe systems was studied; the defective functioning of some feeding valves has been studied and the process of injection moulding during only a few seconds has been visualized (by radiographing the metal moulding form).

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RESEARCH INSTITUTE FOR MICROELECTRONICS (MKI)

The Institute for Microelectronics (established in 1981) has continued its work on data storage using magnetic bubble memory devices, on semiconductors and on mask production. In addition, there was research in new directions in support of R&D activity, in pursuit of an understanding of the mechanism of technology and, in general, into a many-sided exploitation of our experimental capabilities. Considerable progress was made in development of equipment serving automatization of basic technologies.

In the field of bubble memory devices, the main achievement was a casette-type memory device. This will be reviewed separately. Czochralsky-grown gallium gadolinium garnets (GGG, for bubble devices) and barium germanate (BGO, for scintillation counters) were investigated to understand formation mechanismus of as-grown defects. As does calcium, magnesium decreases dislocation density, but its distribution is less homogeneous. It was shown that large fluctuations in temperature are responsible for as-grown precipitates. For BGO fluctuations amounting to 30 ^{O}K were experienced. These were caused by hydrodynamical instabilities of either Reyleigh-Taylor or Conette type.

Crystals used in magnetic bubble devices are ideal materials for the study of magnetic phenomena in general, as most theories apply perfectly to this case. Furthermore, these crystals being transparent, the domains are visible. Using a sampling laser stroboscope (0.2 ns time resolution, 0.4 μm spatial resolution), the process of domain nucleation was studied and saturation of the velocity of wall motion was established. Successful measurements were made of domain motion and deformation in a memory device driven by 100 kHz field. We were able to explain the large coercivity force in YIG type epitaxial thin films. One reason was the unevenness of the surface, but the dominant cause is a 50 nm periodical structure (so-called spinodal decomposition), which was observed in TEM for the first time. A non-negligible macroscopic contribution comes from interfacial stresses at the substrate thin film boundary.

Activity on custom oriented integrated circuits was also pursued. The newest achievements will be reviewed in a separate chapter. This "integrated system" will be developed for design engineers and is adapted to their way of operation. The system is integrated also in that it contains earlier programs, if fitted to individual properties of adjoining computer and shares the job between small and large machines. It is easy to expand the program package and interfaces are included to accept other programs.

The n-MOS circuit technology was improved and adapted to functional devices. Optimized, low-resistivity interconnects were made of polysilicon. In addition, a metal gate CMOS technology was developed and conditions were set to yield proper circuit parameters. Doping by ion implantation was followed by a heat treatment. In most cases we were successful in employing our earlier procedures. Thus aluminium deposition with a magnetron source was readily applicable for both CMOS and n-MOS technologies. A good yield was achieved for the circuit 4011.

Gate matrix circuits were produced both with CMOS and n-MOS technologies. The CMOS technology was transferred to the industry, the Enterprise for Microelectronics, Budapest, where extraordinarily high yields were achieved right away.

In cooperation with the Work for Mechanical Measuring Gears, a silicon based pressure sensor was developed, again with very good output yields. A complete wafer technology is now running in our laboratory.

Results of research on titanium silicide were incorporated into our wafer technology reducing the resistivities of interconnects by an order of magnitude compared with poly-Si. Combined ion and plasma etch procedures resulted in a structuring of titanium silicide which preservers dimensions.

We continued our work on a 256 kbit bubble memory device. Using a patented version of double-layer photolitography, we were able to produce 1 μm lines in a 1-2 μm thick resist layer. This enables us to produce high resolution patterning of metals and semiconductors in great variety.

Photolitography of poly-imide layers was developed for a chemical produced in the Institute for Synthetic and Rubber Materials of the Technical

University, Budapest. Experiments were made to study the use of this material as protecting layer for semiconductor devices and as an intermediary insulating film in bubble memories.

A low-pressure chemical vapour deposition system was built, yielding layers with properties equivalent to those produced in known professional equipment.

To the optical mask laboratory, established in 1980-81 to meet R&D demands, a new section was added for visual control. There the comparing of masks, the control of dimensions as well as some repairs can be made on a high level. The laboratory is thus able to fulfil the most stringent demands in mask production. During the past year, more than 150 mask sets were produced for our institute or for customers, such as the Enterprise for Microelectronics and the Institute for Technical Physics. From a technical viewpoint, our peak achievement was a set of masks for Institute for Technical Physics which features a master set of a GaAs MESFET with a 0.8 μm resolution. Another considerable achievement were mask sets for a 256 kbit bubble memory chip and for a 4011 n-MOS RAM. This latter involved in some layers nearly 50000 exposures (35-40 hours uninterrupted operation), which shows extent of our efforts to improve the reliability of the original system.

In the field of materials science of semiconductors, there were extensive investigations of implanted amorphous silicon layers. This time ESCA, UPS methods were also used leading some conclusions on complex structure of the layers. We found that the implanted amorphous state is composed of two kinds of structure, each having different electronic structure. The two states behave differently during thermal annealing.

Studies on silicide systems were reviewed in detail in the previous yearbook. During 1984, the electronic structure of the titanium silicide was determined, again with UPS. Jointly with the Department of Materials Science and Engineering of Cornell University, further work was done to compare ion mixing and pulsed ion beam annealing. Supported by experiments on the Al-Fe thin film system, the thermal behaviour of the pulsed ion beam treatment was established. In another joint project, with the Institute of Semiconductor Electronics of the University of Aachen, the oxidation properties of $TiSi_2$ were measured. On top of the silicide a layer of SiO_2 is formed during thermal oxidation, leaving the silicide unaltered. However, if TiO_2 was present on the $TiSi_2$, the thermal oxidation process was inhibited. This shows that the transport of oxygen through TiO_2 is extremely slow.

During 1984 work on ellipsometry progressed to the point where investigators can determine the thickness and degree of amorphousness of implanted surfaces, both silicon and other materials, e.g. GaP. The technique looks promising also in practice as a non-destructive method. The real thickness of the layer was measured by backscattering and channeling in a tilted detector configuration. Degrees of amorphousness between 10 and 100% are measurable.

Two important pieces of equipment began operation this year: an implanter with energies up to 500 keV for singly charged ions, and a laboratory model of a system for rapid annealing using halogen lamps. First experiments were on ion mixing of silicides and on annealig of implanted amorphous layers.

The group working on logic simulation ended a successful year with an international conference organized here and with results which will lead in 1985 to the first version of a mixed mode simulation program.

The Technical Department provides the technical background for microelectronics research activities. A minor part of the work of this department is the maintenance of all electronic equipment used in the institute. The major part is the development of new devices and equipment and the solution of problems in the automatization of measurements. In the last two years we have designed and produced about 40 devices and items of equipment.

The development of Single-Crystal Growth System has been continued. In addition to the development of several units (e.g. differential driving mechanism, crystal weight measuring unit, low temperature growing device) we started the development of the electronic part of the Czochralski-type Crystal Growth System. The development program of the Crystal Growth System suggested the necessity of a high precision electronic balance. The balance we developed has 10 kg measuring range with 0.1 g resolution. In addition to crystal growth application it is suitable for universal weighing.

Another area in which we are active is the development of ion-beam devices. For the SAFI type ion-implanter developed earlier a fully automatic wafer processing station was developed. Research on a pulsed ion-beam technique also was begun. Several laboratory data processing systems have been produced. These microprocessor based systems can be fitted to local conditions to solve the problem of automatization of measurements.

*

METAL GATE CMOS TECHNOLOGY FOR THE REALIZATION OF UNCOMMITTED LOGIC ARRAY AND CATALOGUE CIRCUITS

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1. ON CMOS CIRCUITS, IN GENERAL

Realization of complementer (consisting of p- and n-channel transistors - CMOS) integrated circuits became possible in the middle of the sixties.

Because of their known advantages - low power consumption, insensitivity to noise, wide range of power supply - CMOS first was applied in clock circuits and space electronics. Years later, in the middle of the seventies, there appeared CMOS based calculators and microprocessors containing a higher number of elements. In these circuits, which use silicon-gate technology and oxide isolation, the disadvantages of the traditional CMOS structure (namely remarkable well size) have been avoided.

In the end of the seventies, after the 'heroic period' of microprocessors, for the sake of faster and more versatile satisfaction of the users demands all kinds (bipolar, MOS, CMOS, CML and so on) of so called semi-finished circuits ULA (= uncommitted logic array), began to proliferate. Since in case of ULA the circuit is 'prepared' by the user by planning the metallisation photomasks, it is neccessary to have a certain redundance of the half-finished elements (cells). The reason for this is that it is impossible to imagine an arrangement of cells being optimal for all users. This leads to the neccessity of longer conductive lines with less resistivity. Low resistivity is especially important in case of periphery circuits (the ones that ensure the TTL compatibility of the CMOS elements) because of their lengthy gate electrodes.

2. SOME QUESTIONS OF CONSTRUCTION AND TECHNOLOGY

In order to obtain the neccessary threshold voltage both for n- and p-channel transistors ($|V_{Tp}| \cong |V_{Tn}| \cong 1$ V) after various annealing procedures, silicon wafers of (100) orientation, 12 ohm cm resistivity were chosen as starting materials, a choice made on the basis of technological considerations and computer modelling, see ref. [1]. In this case due to the low value of the impurity concentration ($N = 4 \times 10^{14}$ cm^{-3}) the switching time of the circuit decreases at a higher risk of punch-through between sources and drains of the p-channel transistors. The other consequence is the lowering of the breakdown voltage between the p^+ and n^+ diffusion stripes. The smallest allowed distance between these stripes, as calculated for the case of highest supply voltage (20 V) is 2.8 μm. Our calculations are based on the so called abrupt junction approximation, which results in the lowest breakdown voltage (worst case).

The minimum distance d between the p^+ source-drain areas (the channel length) with no punch-through at drain source voltage V_{DD} = 20 V is given by

$$d = \left(\frac{2\varepsilon}{qN} V_{DD}\right)^{1/2}, \tag{2.1}$$

which gives 8.1 μm. Here, ε is the dielectric constant and q the electron charge. In practice the situation is better, because of the presence of positive oxide charges the electron concentration at the surface is higher than in the bulk material. The flat-band voltage of the gate oxide is around -0.3 V and the corresponding surface potencial is $\psi \cong 0.08$ V, see ref. [3], so the electron concentration at the surface is:

$$n_s = n_o \exp(q\psi/kT) = 8.7\text{x}10^{15} \text{ cm}^{-3}$$

where n_o is the electron concentration in the bulk. According to this value the minimum source-drain distance (see eq. [2.1]) is 1.7 μm, which compared to 8.1 μm is more favourable. In the case of n channel transistors there is no similar problem because at the surface of the p-well the hole concentration is two orders of magnitude higher than the electron concentration at the surface of the silicon single crystal.

The conclusion is that in the construction abiding of distances has a critical role (the punch-through voltage is proportional to the square of the source-drain distance). Because of this all critical photolitographical operations (patterning the p^+, p and n^+ layers) are carried out on a relatively thin (0.3 μm) silicon dioxide layer, so the error in the patterns' distance is as low as 2x0.3 = 0.6 μm. After the critical photolitographical procedures the oxide thickness is increased by CVD upto about 1.5 μm so the threshold voltage of the parasitic transistors (field threshold voltage) would be lower than the maximum supply voltage.

3. VERTICAL STRUCTURE OF CMOS TRANSISTORS

It has been our task to determine the depth of the p-well and the dose of implanted acceptor impurities - in our case the dose of boron. For the junction depths the following relationship must be satisfied:

$$x_p - x_n > x_{d_1}^{max} + x_{d_2}^{max} \tag{3.1}$$

That is the distance between well-substrate and drain-well junctions must be greater than sum of depletion layer thicknesses in the p-well at a

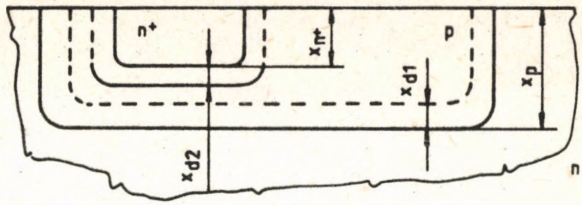

Fig. C-1
Cross-section of the p-well

maximum voltage. Taking for the threshold voltage V_{Tn} = 1 V, and using the simple expression

$$V_{Tn} = V_{FB} + 2\psi_B + \frac{1}{C_{ox}}\{2\varepsilon qN(2\psi_B)\}^{1/2} \tag{3.2}$$

where ψ_B is the bulk potential and C_{ox} is the specific gate capacity, we obtain $N \cong 10^{16}$ cm^{-3} for the boron concentration at the surface of the p-well. In these circumstances the maximum allowed flat-band voltage V_{FB} between the aluminium gate and the p-well is V_{FB} = -1 V. The implantation dose Q of boron and the junction detph of the p-well X_p are determined so that, on one hand, the maximum of boron concentration after drive-in diffusion must be equal to 10^{16} cm^{-3}, and on the other hand, the maximum of the depletion layer thickness at highest supply voltage should satisfy relationship (3.1). The depth profile of boron, implanted with a dose

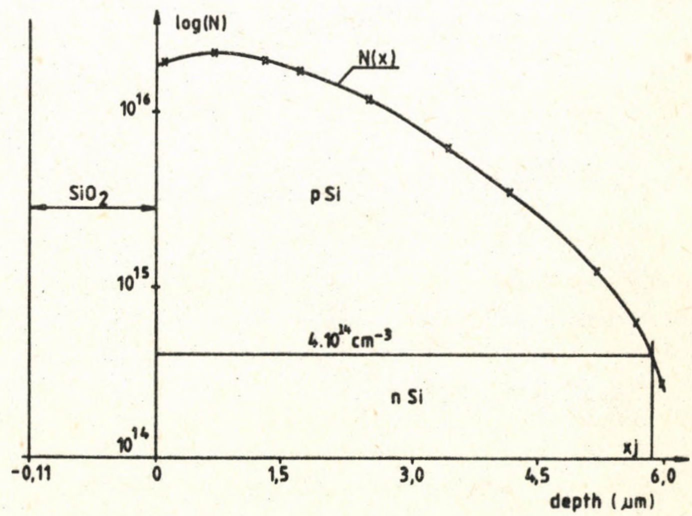

Fig. C-2
Boron profile after drive-in diffusion

of $6.9x10^{12}$ cm^2, obtained by computer simulation is shown in *Fig. C-2*. It can be seen that in this case the p-n junction depth is 5.8 μm and the concentration at the Si/SiO_2 interface is $2x10^{16}$ cm^{-3}. The calculated sheet resistivity of such a p-well is 2.7 kohm/□. The transfer and current characteristics of the inverters of the ready circuits are shown in *Fig. C-3*.

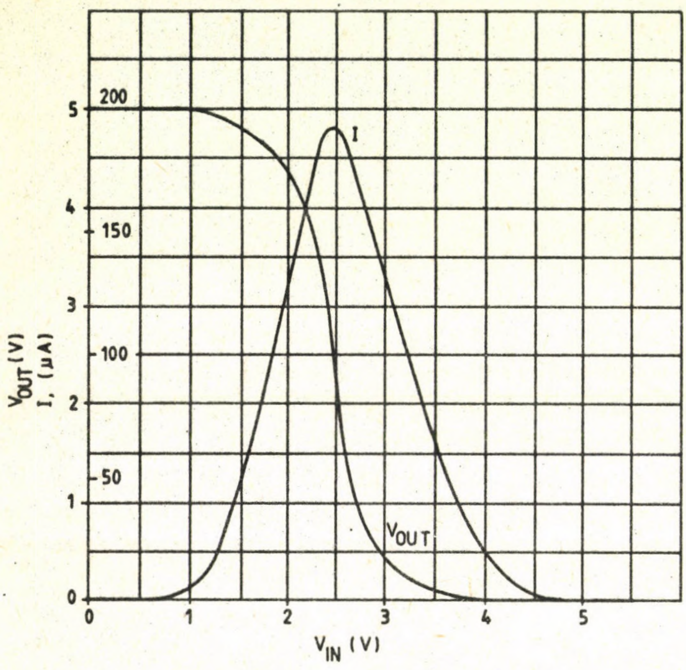

Fig. C-3

The inverter characteristics

4. SCHEMATIC REVIEW OF PREPARATION OF METAL- GATE CMOS CIRCUITS

One of the characteristics of the technology is that it contains three implantations: high-dose implantation of source and drain areas with boron and phosphorus ions and implantation of p-wells with a middle level of boron dose. In the case of implantations the masking material is photoresist spun on SiO_2 (the SiO_2 thickness is 0.05-0.3 μm).

All oxidations are done in a dry atmosphere and the patterning is carried out using a wet photolithographical procedure. At field areas an additional SiO_2 layer is deposited onto the 0.3 μm thick oxide layer using standard chemical vapour deposition (CVD). The resulting SiO_2 thickness is 1.3 μm. The 1.2 μm thick aluminium layer is deposited using a magnetron evaporation system, which is advantageous from the point of view of the tearing resistance of the aluminium conducting lines. The structure formed by these main technological steps can be seen in *Fig. C-4*.

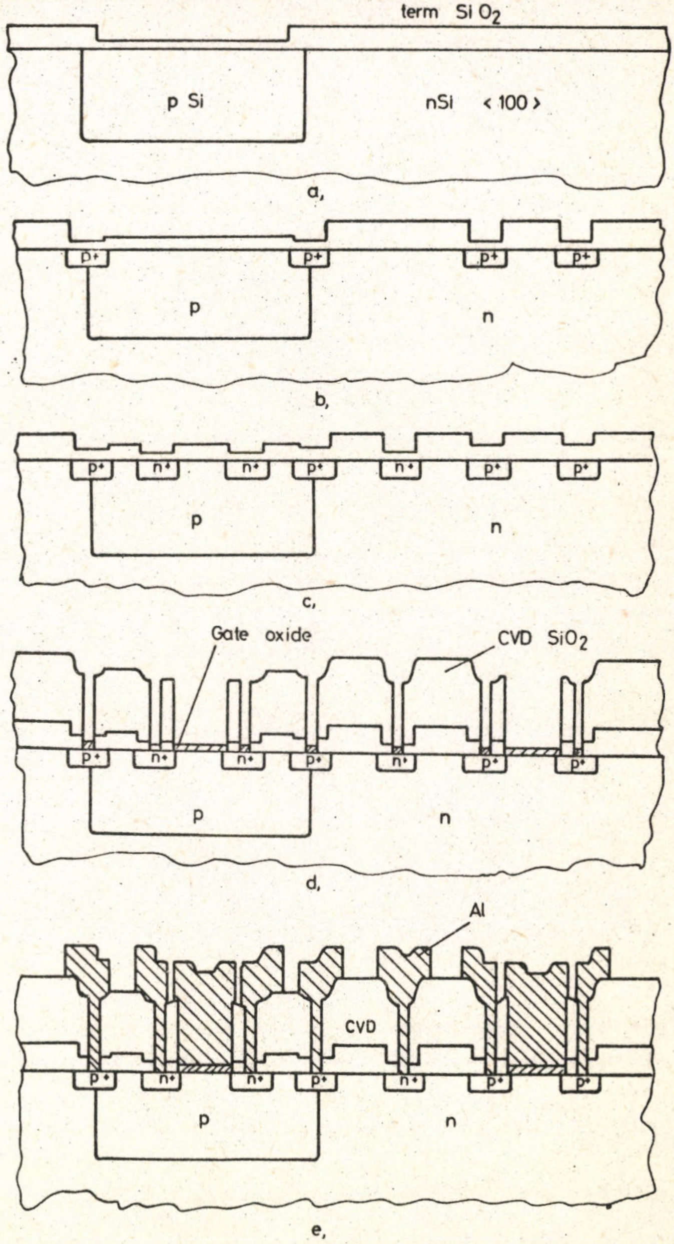

Fig. C-4

The structure formed by the technological steps

5. APPLICATION OF CMOS TECHNOLOGY CG (CMOS GATE) ULA

The CG family consists of three members: CGA, CGB and CGC. Their semiconductor device structure and transistor parameters are identical and they differ only in the chip size and number of transistors. For this reason, the layout of the smaller versions - for example of the CGA - can be applied for CGB and CGC. The same is true for circuit units of the cell library.

The circuit design can be carried out either by "hand" or by computer. In the first case the layout of the circuit is made by 2 mm wide sticky tapes (- similar to PC board technology) on a black-and-white film with 200 X magnification of the chip.

The main parts of the matrix cells and input/output units (- the gate electrodes and contact areas -) are printed on the film in advance. The end of the sticky tape and the sticky patterns of library elements must be positioned with an accuracy of 0.6 mm at these predefined areas. If the user is not satisfied with the cell library elements (which are at his disposal also as sticky patterns) he can also redesign the basic circuit according to his own conception. While cheapness is the main advantage of the design by 'hand' at the same time it demands a great attention to avoid mistakes during the design procedure. The computer technique, though more expensive, lacks such drawbacks. Table 1 summarizes data of the CG family.

Table 1

	CGA	*CGB*	*CGC*
chip size (mm^2)	*3.2x2.7*	*3.5x3.4*	*4.5x3.4*
number of cells	*56*	*81*	*108*
number of TTL drivers	*14*	*18*	*18*
number of MOS drivers	*16*	*18*	*24*
number of bonding pads	*32*	*38*	*44*
number of pullup transistors	*32*	*38*	*44*
number of inverters	*168*	*243*	*324*
number of 2 input gates	*140*	*202*	*270*
number of 3 input gates	*84*	*121*	*162*
number of 4 input gates	*56*	*81*	*108*

All array-cells consist of 5 p- and n channel transistors and 7 underpasses.

In the input and output cells the pullup transistors are positioned near the bonding pads and their source outputs are connected to the supply voltage line. The user should only connect the drain outputs to the pads and the gate electrodes to the ground line. In such a way, the incoming TTL level automatically will be pulled up to the driving level of the CMOS inverter. The TTL drivers can be loaded with four TTLs and the buffers can take one TTL load. In *Fig. C-5* the metallization mask of a CGB variant circuit manufactured for industry is shown.

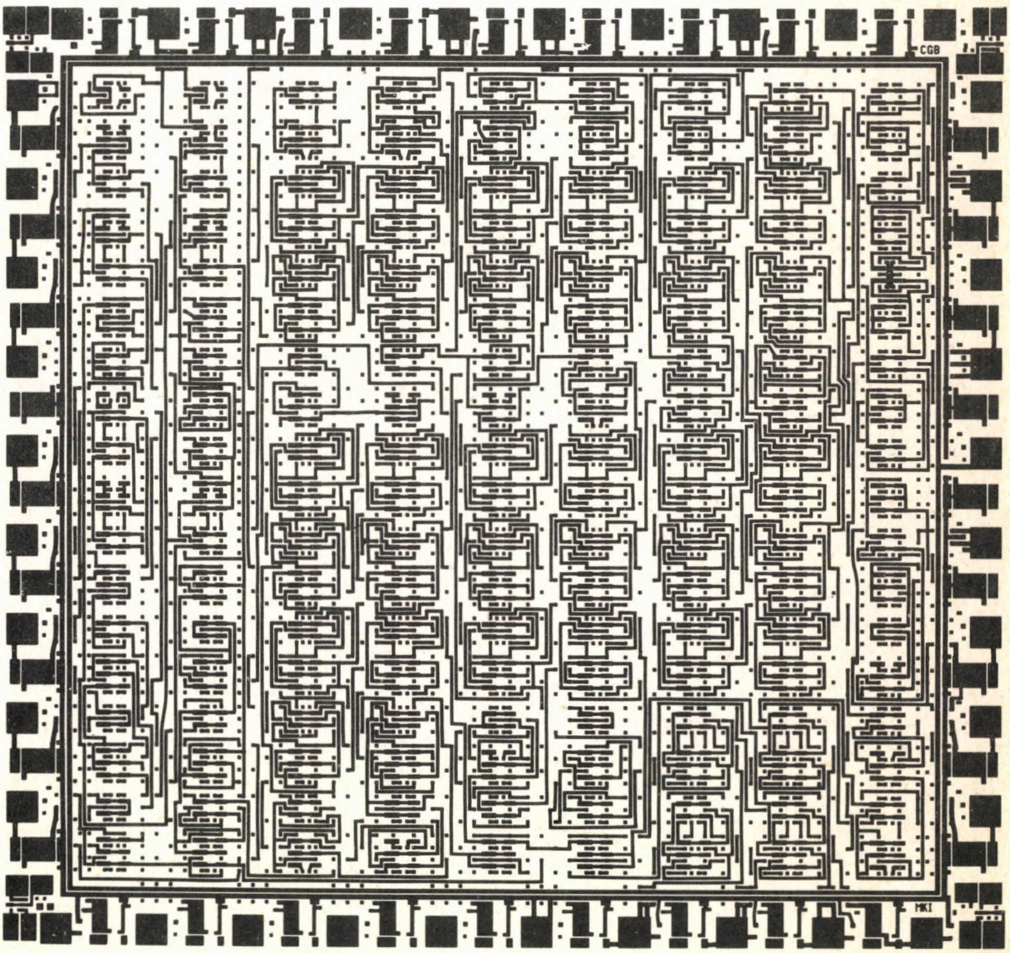

Fig. C-5
Metallization mask of the MRI circuit

It's design has been carried out by hand, and as it is clearly seen, almost all (98%) the cells (or transistors) are used.

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BUBBLE MEMORY CASSETTE CONTROLLED BY CUSTOM-DESIGNED INTEGRATED CIRCUITS

G. Zimmer, I. Eördögh, G. Nagy. P. Szőke and L. Bodócs

A mass memory with a changeable data carrier, a maximum capacity of 256 kbits, and CRC protected information contents has been developed based on the memory device type MBM 256 made according to the technology worked out in the KFKI. The storage system can be programmed universally and also used as an intelligent terminal. The realization of the instrument is facilitated by the fact that most details - beside some standard LSI circuits - are integrated in two custom designed integrated circuits which could be eventually produced by the Microelectronic Components Company of the Telecommunication Cooperative and the KFKI.

1. INTRODUCTION

In computing technology directly processed data are in an operative memory (RAM) the capacity of which is not too great, but in which the data are quickly accessible. These semiconductor memories are easily joined to the processor, but if there should be a failure in the power supply, the stored information will be lost.

In most cases results are permanently stored in relatively slow big capacity magnetic disc or magnetic tape mass memories. These are rather inconvenient, because they are fairly big and contain moving components which cannot be produced directly by microelectronic methods. They are, at the same time, indispensable, since the magnetic storage preserves the information for a practically unlimited period. There is, however, a difference of four orders of magnitude between the access time of RAMs and magnetic mass memories.

The bubble memory fills the gap between semiconductor storage - generally faster than 10^{-6}s - and magnetic mass memory - slower than 10^{-2}s. With respect to access time and capacity, the bubble memory falls between quick and slow memories, and similar to other types of magnetic memories, preserves the information for an unlimited time. It can be produced by microelectronical technology and doesn't contain moving mechanical components.

2. BUBBLE MEMORY CASSETTE TYPE MBM 256

The bubble memory cassette is a shift register system based on the magnetic principle, the stages of which contain a logical 1 or 0 according to the presence or absence of a magnetic bubble in the stage. The bubble itself is a domain in the magnetic layer endowed with the necessary features, which has magnetization contrasted to that of its environment, and which can be generated or collapsed as desired. We would like to mention, without going into details concerning the working of the bubble memory, that, the charging of the shift register (that is the generation of the bubble) and the shifting of the information (that is the bubble) or its eventual copying from one register to another happens via miniaturized conducting loops, in which at the right moment current is driven to create local magnetic fields. The information is shifted along the register also by magnetic fields, but the current in the macroscopic pair of coils marked X and Y in *Fig. C-6* shifts all stages of all registers simultaneously.

The bubble memory type MBM 256 operates on the major-minor loop organization. This means that 282 independent shift registers 1025 bits long (called minor loops), which are each one closed in themselves, have the function of information storage. The open register used for the input of information, one of the major loops, is connected with the storage loops via transfer-in gates. The second open major loop, connected via transfer-out gates to the block of minor loops, leads the information to be read to the detectors.

The stored information can be written into and read from the memory in blocks containing as many bits as memory loops, and the number of blocks is equal to the number of bits within one memory loop. The major - minor loop organization shortens considerably the access time of the information blocks and lessens the influence of failures that occured during the technological process. If there is no technological failure in the writing and reading major loops, the surface of which is small compared to the whole chip, the defective storage loops (supposing that their number is relatively low) can be left out via the software, when the memory module is used. The position of defective loops is ascertained by the memory testing procedure. During operation no bubble is written into the defective loops and bubbles eventually read out of them are left out of the useful bit series.

The 256 kbit storage capacity bubble memory, MBM 256 contains 282 storage loops and each of these have 1025 bubble positions. The maximal length of data blocks in 282-14-r, where r is the number of defective minor loops. CRC bits for detecting and correcting accidental failures occupy 14 bit positions.

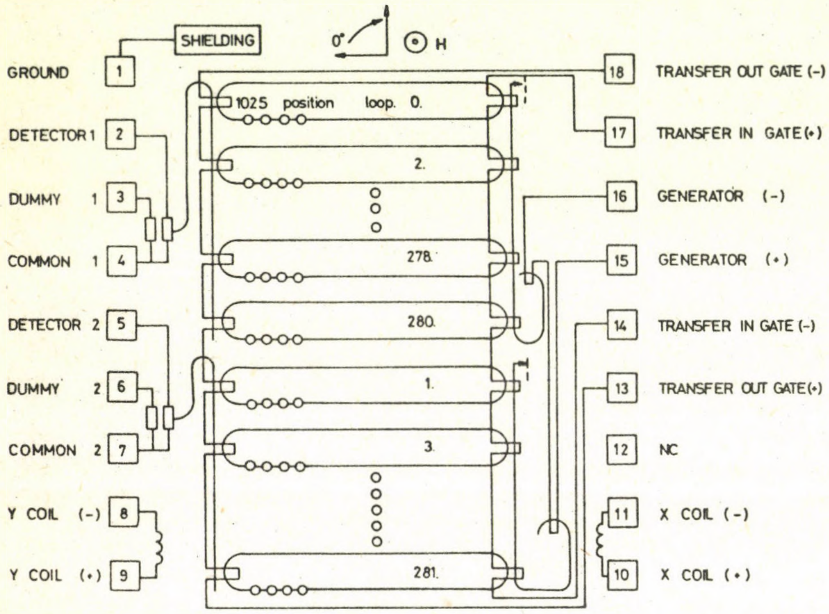

Fig. C-6

Architecture of the 256 kbit bubble memory

Figure C-6 shows the sketch of the 256 kbit bubble memory chip. The surface of the chip is divided into two identically structured parts; the even bits of the information blocks are in one half, the odd ones in the other. Both halves contain a generator and a writing major loop with transfer-in gates, a storage field with storage loops and a reading major loop with transfer-out gates and a detector. The transfer-out gates have two functions: they either load the next data block into the major loop leading to the detector and leave space empty in the storage loops, or they divide (replicate) bubbles moving through them: i.e., they send one bubble back to the storage loop and load the other into the major loop. Thus, reading is possible with the preservation of the stored information blocks.

In the arrangement shown in *Fig. C-6* both generators produce the same data block in parallel, but these are written into the two major loops with a shift of one position. As the transfer-in gates are activated at the same time, because of the one bit shift half of the data block (every second bit) will be written in one, while the other, complementary half of the data block into the other part of the chip. In the same way, during read out the transfer-out gates are activated at the same time, the two complementary parts of the data block appear in the major loop in every second bit position; but on the way to the detectors via the built-in one bit difference and joining the signals of the two detectors, the original form of the data block will appear in the common output.

3. THE CASSETTE MEMORY UNIT

The information carrier is a changeable bubble memory type MBM 256 built into a plastic cassette. The instrument can also be used, with the help of a built-in monitor routine, as an independent, intelligent terminal.

It has a block data structure. One cassette contains 1025 data blocks, the length of the blocks changes flexibly depending on the useful capacity of the bubble memory built into the cassette. The user, however, does not have to know the inner structure; all is done by the built-in software.

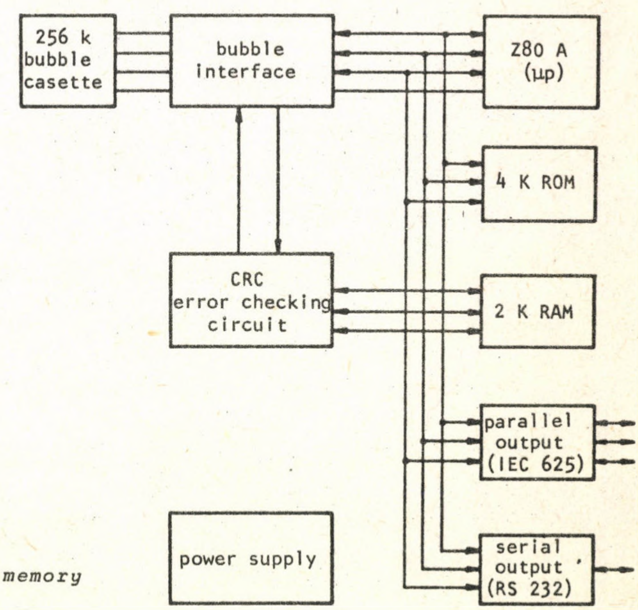

Fig. C-7

Block diagram of bubble memory cassette system

Figure C-7 shows the structure of the memory consisting of a Z80 based microprocessor, connected standard peripherical circuits, the special electronic circuits controlling the bubble memory, the CRC circuits correcting accidental errors and a power supply ensuring the correct sequence of on and off switching of the voltage.

The instrument can also be accessed by a RS-232 serial interface channel; it can be connected, for example, to a standard VIDEOTON display unit. The rate of data transfer is limited (maximum of 9600 baud). It is easy to activate the monitor routine through this channel.

The parallel input output channel processes standard (IEC) signals. Both in the case of serial and parallel access data are transferred between the environment and the buffer memory of the micromachine and, between the buffer memory and the bubble memory. A microprogramme ensures an unambiguous correspondence between the logical and physical address of the data blocks incoming one after the other. Another microprogram ensures the zero-setting of the memory after a sudden power failure and the search of the data files. The micromachine and its parts can be cheaply and simply constructed from standard LSI components.

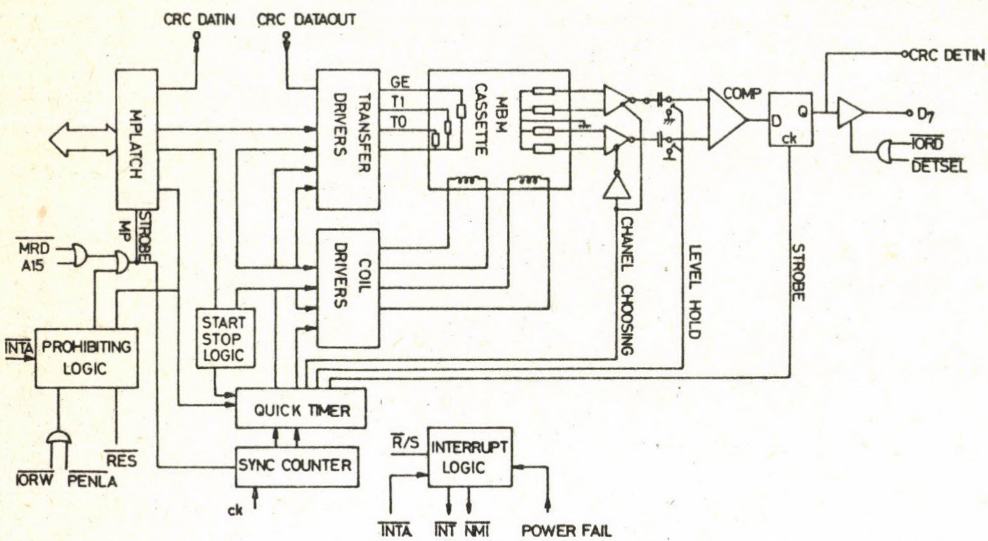

Fig. C-8

Block diagram of the electronic system

Figure C-8 shows the principle scheme of the electronics directly controlling the bubble memory. The circuit is connected with a Z80 bus, and the microprogramme command arriving through this bus ensures the signals for the coils to shift the information and the series of control signals to produce current for transfer-out and transfer-in gates. This stage also converts the signals of a few millivolts, created during the sensing of the bubble, to TTL level.

MPLATCH is a mirror register of the accumulator of the processor. The microprogramme commands are written into this memory by means of exactly timed memory reading cycles organized into an infinite cycle. The system can continue its work by an interrupt of this infinite cycle.

The microprogramme commands follow each other exactly in 64 clock cycles. Complete synchronism is reached via a synchronizing signal derived from the strobe signal; this means the quick timing unit is zero-set at the necessary intervals.

The START/STOP logic ensures that the current of the coils driving the bubbles along the shift register filled with bubbles can be switched off under all circumstances when shifting is to be finished.

The prohibitive logic ensures that MPLATCH can be activated only while the microprogramme is running; this prohibition is induced from the INTA answer, given to the INT interruption signalling the end of the microprogramme.

The INTERRUPT logic also controls the POWER FAIL signal. If the power should fail during a bubble shifting period, the microprogramme is stopped only when the shifting is finished.

Bubble detection is done with the clamping method, which is generally used in analogue signal processing. In the circuits of the detector - where the signal is measured in millivolts - considerable noise is caused in an inductive and capacitive way by the magnetic fields shifting the bubbles. This noise can be eliminated to a great extent if the capacitances shown in *Fig. C-8* are charged to the potencial that existed before the appearance of the signal. The comparator senses only the useful signal and writes it into the output data storage register. There it is stored until processed by the DETSEL and IORD signals of the processor.

The movement of the bubbles and, especially the working of the bubble detector is disturbed by magnetic and electric fluctuations and noises. Not too often (say once in every one thousand million readings) faulty information may be written in the data store. The bubble memory cassette has a CRC (cyclical redundancy check) data protection system. The process, the details of which cannot be described here, is based on the so-called Fire-codes and needs in every data block 14 bits of plus information (check bit) to be able to correct every block which has maximum one error burst of 5 bits. The process can also detect bursts not longer than seven bits. During operation polynomials have to be divided by each other; the 1's and 0's following each other in the data flow represent coefficients of increasing powers of x. This polynomial must be divided with an expediently selected polynomial, in our case $x^{14}+x^{11}+x^9+x^5+x^2+1$. So as to make the process faster and the load on the processor less, this happens via the hardware, in a CRC circuit.

The generation of checking bits, correction and detection of errors can be controlled by words put in via the control port. When writing in, the data enter the bubble memory and the dividing circuit at the same time. After this the CRC check tail is shifted into the bubble memory. When reading (detecting), the data block completed with a CRC tail enters the data block storage register and the divider at the same time. If the data block is correct, this divider is empty. If the data block contained an error, the circuit shows it, and correction follows depending on the content of the divider. The system itself does not signal beforehand whether some special errors will be correctable. This means that the corrected data sequences will have to be checked again. As the probability of errors is very low indeed, this extra time is only seldom required and the access is only slowed to a negligible extent.

4. SEMI-CUSTOM-DESIGNED IC IN THE MEMORY CONTROL

The number of packages, the power consumption and testing time of the bubble memory control circuits could be several times higher then those of the micromachine part, even though the greatest part of the transistors is found in the microprocessor and the connected standard LSI circuits. The same can be said about CRC circuit. So as to make the production of the bubble memory cassette data recorder practically possible, these circuits, or at least their greater part, must be integrated.

As it is known the Telecommunication Cooperative and KFKI have founded an association to plan and produce gate-array (matrix type) circuits. Making use of the facilities of the Microelectronic Components Company, we planned the CMOS integrated circuit which can replace the logical part of the bubble controller. This circuit replaces about 15 TTL SSI/MSI circuits and contains the complete bubble fast controller (except for the analogue sensor-amplifier and the power supply).

The use of the cyclical redundancy code in magnetic peripheral memories is neither unusual, nor unknown. Several such custom-designed integrated circuits are on the market. However, we had to plan a special circuit for the bubble memory, see *Fig. C-9*, as the length of the blocks cannot be chosen freely, they follow from the structure of the memory component we have to work with, in the fixed data group. The code which gives the best results in this special application was selected after a

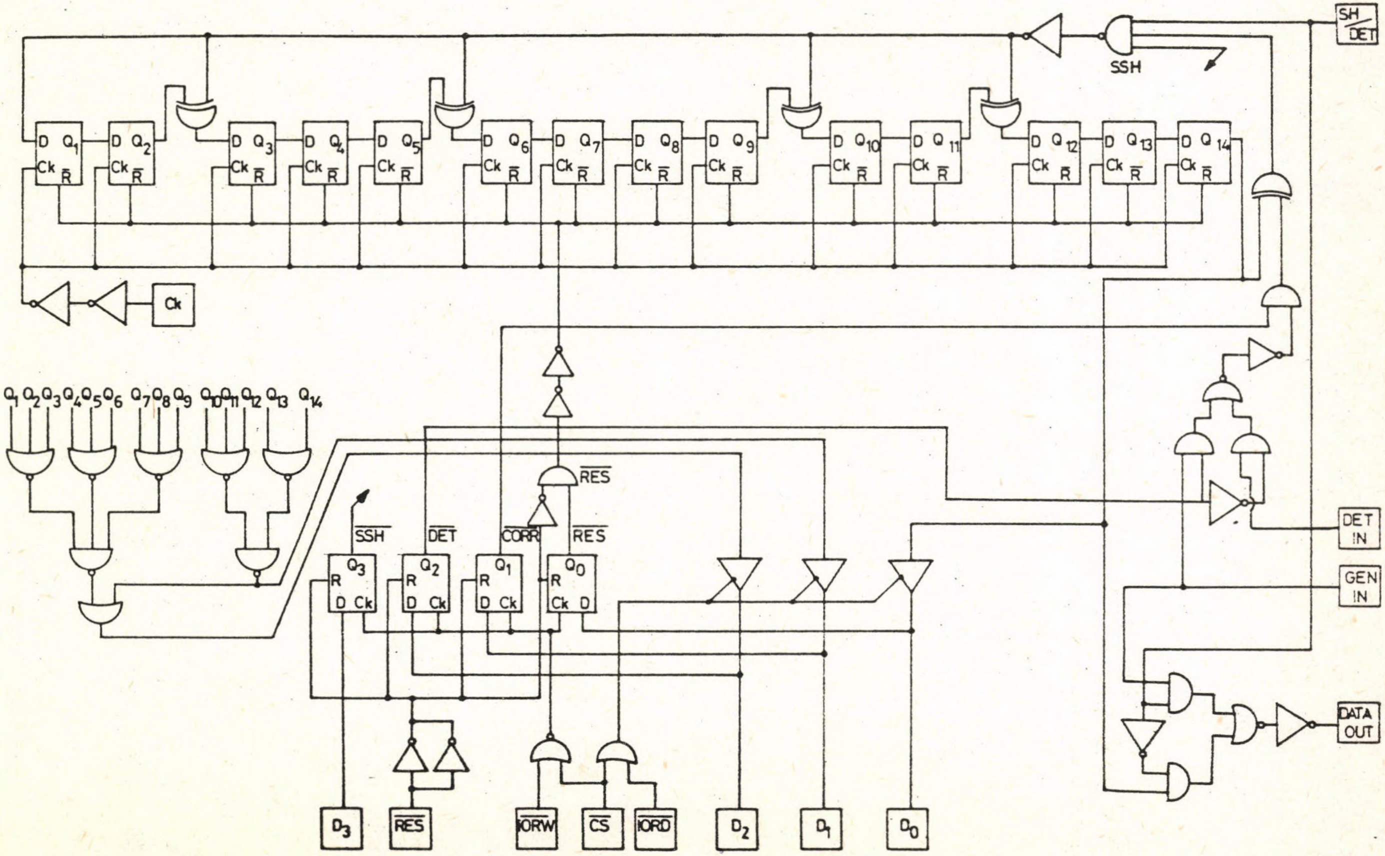

Fig. C-9

Schematic of CRC circuit

detailed analysis of the Fire-codes. An integrated version of this circuit has been also completed, again by making use of the facilities of the Microelectronic Components Company and our institute. *Figure C-10* shows the layout of the metal layer of the semi-custom designed integrated circuit. As a comparison, *Fig. C-10a shows a* version produced by Microelectronics Component Company on an imported wafer, and *Fig. C-10b* the version on a CMOS wafer, planned and produced in KFKI. The bubble memory casette system is shown in *Fig. C-11*.

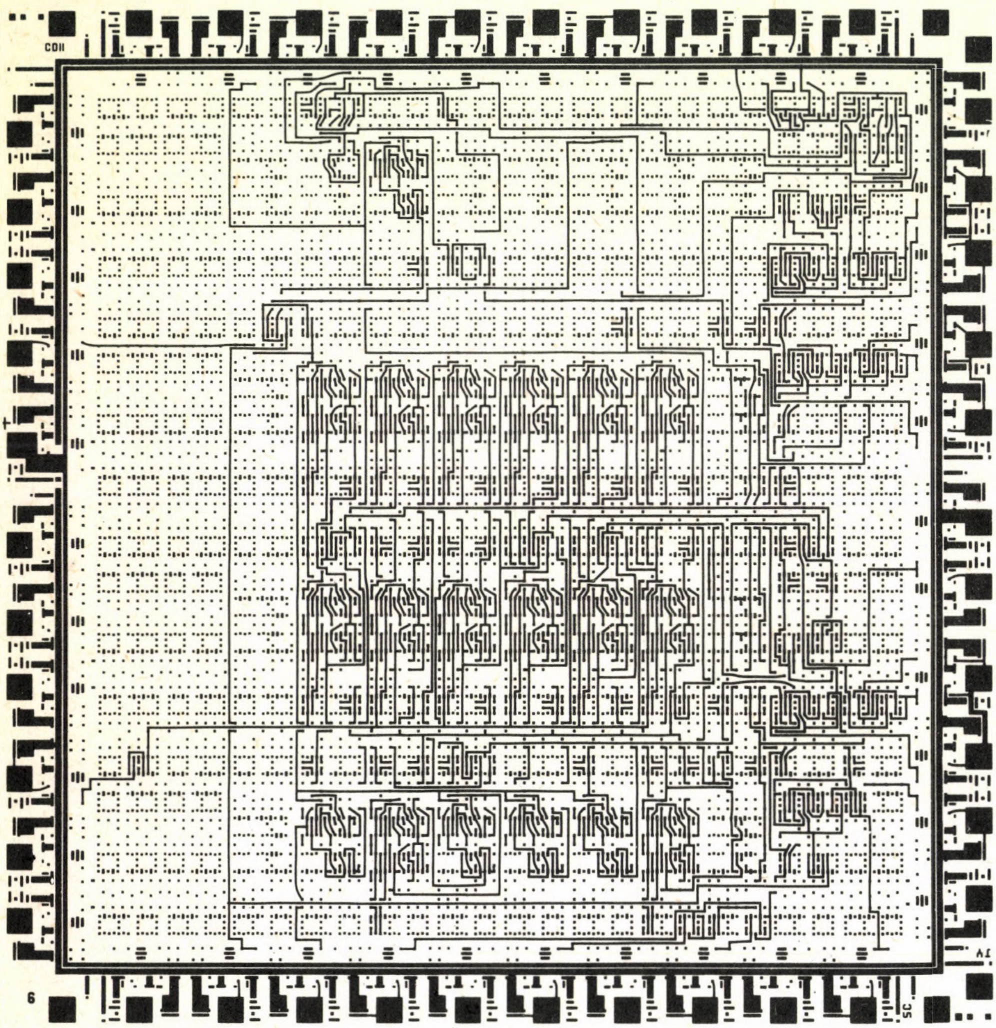

Fig. C-10a

Metal layout of CRC circuit on a MEAT (Microelectronic Components Company) wafer

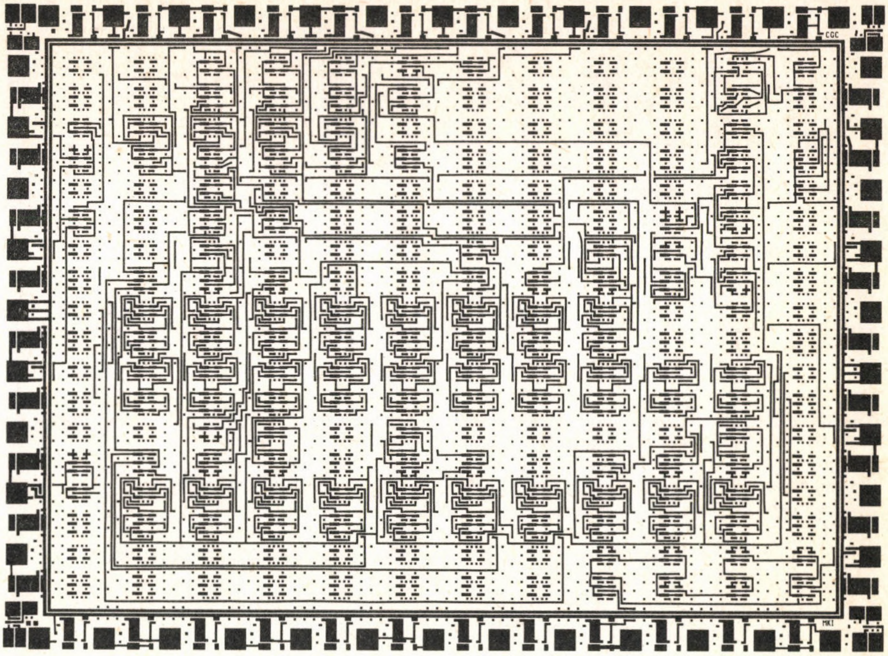

Fig. C-10b

Metal layout of CRC circuit on a KFKI wafer

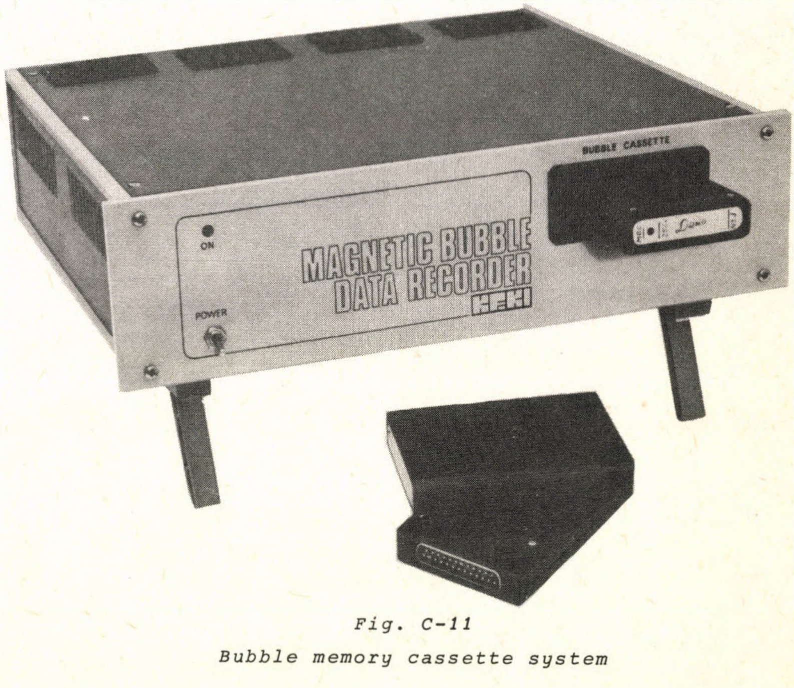

Fig. C-11

Bubble memory cassette system

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INSTITUTE FOR ATOMIC ENERGY RESEARCH (AEKI)

The activity of this institute has been shared among three main tasks. Whereas extensive work has been devoted both to the launching of the Paks Nuclear Power Station and the planned reconstruction of the institute's research reactor, new instruments and methods were also developed for the benefit of the National Microelectronics Program. The scientific background of these and related works includes research in neutron physics, reactor safety as well as renewable energy sources.

REACTOR PHYSICS AND NOISE DIAGNOSTICS

The primary goals of reactor physics research are the development of calculational and experimental methods for reactor operation purposes, the performance of design and survey calculations and the development and application of monitoring and early warning techniques.

Core calculations are developed through detailed comparisons with specially designed experiments. The experiments are carried out on the zero-power reactor ZR-6 as part of an international collaboration. The experiments include measurements of critical parameters, macroscopic flux distributions and spectral parameters in various core configurations at different temperatures. The first group of such experimental results has recently been published as Volume I of a larger publication covering more than ten years of activity (see List of Papers, N° D18).

The core and frame of a reactor calculation system of modular construction has been written for the automatic handling of complicated, multiprogram calculations. Theoretical results have been published in the field of the finite difference and coarse mesh approaches to the diffusion approximation, and new programs using these results have been written. Design calculations and evaluations have been carried out in connection with the compact storage of burnt fuel assemblies at the Paks Nuclear Power Station, the reconstruction of the WWR-SM research reactor and a zero-power reactor to be built in Cuba.

The neutron irradiation of the Paks reactor vessel has been measured in order to facilitate the evaluation of its possible degrading and expected lifetime. Other calculational activities were connected to special problems of shielding and the occurence and migration of radioactivity in the cooling water.

A core performance monitoring system (VERONA) has been developed and installed at units 1 and 2 of the PAKS power station. It uses a series of in-core and primary loop measurements to calculate important parameters and to show them to the reactor-operators in the form of various display patterns, printed logs and archives.

In the field of reactor noise analysis and reactor diagnostics we have developed new theoretical models for stationary two-phase flow diagnostics and methods for the description of the neutron field caused by in-core vibrations, including the localization of the vibrations. The theoretical models have been extensively studied by numerical calculations and are being compared with zero power experiments and power reactor measurements. Reactor noise measurements are made possible at the Paks Nuclear Power Station by the installation of a special measuring equipment, a result of several years' technical development in the field of low amplitude fluctuation measurements. Reactor-noise measurements are continuously carried out at the power station, and special experiments are being performed at the UR-6 zero-power reactor and in the Rheinsberg Atomic Power Station (GDR). The noise characteristics of various operational conditons are collected and interpreted in terms of the models, and malfunction monitoring algorithms are being developed.

THERMOHYDRAULICS

In the field of reactor thermal-hydraulics there are four groups of results which characterize the research activity: the research and development program for the core thermal-hydraulics of the WWER-1000-type reactors, nuclear safety, an ongoing program to provide for the safe operation of the Paks NPP and the thermal-hydraulic design of the research reactor (which is under modernization).

Critical heat flux, coolant mixing and hydraulic measurements have been performed on the NVH high pressure facility in order to support the development of a computer code which will be used for a detailed core performance analysis of the WWER-1000 reactor.

An extensive computer code safety analysis of the Paks NPP has been completed with special attention given to the WWER-440. Specific problems include natural circulation behaviour and small-, medium- and large break LOCAs. To support the code analysis an integral type test facility called PMK-NVH has been constructed. It is a full pressure primary circuit model of the Paks NPP having a scaling ratio of 1:2070 for volume and power. The facility is the experimental basis for a "Standard Problem" organized by the International Atomic Energy Agency.

A detailed core analysis, using operational data has been finished for units 1 and 2 of the Paks NPP. Special attention was given to the critical heat flux ratios.

Important and valuable results have been achieved in the design of the new core and the emergency cooling systems of the modernized research reactor of this institute.

REACTOR ELECTRONICS

In the period of 1983-84 the largest task of the Department for Computerized Reactor Control was the development of the VERONA on-line core monitoring system. The development is carried out in cooperation with the Reactor Physics Deparment. The goal of the work is to determine the 3D power distribution on the basis of measured in-core data, and to present this information on colour display units in the block control room. The system measures some 700 analogue and about 300 digital variables with 16 sec cycle time. After every measuring cycle the core is evaluated and the corresponding display pictures and logs are generated. The first experimental system begun to operate in the Summer of 1984 in Unit I. At present two identical systems are operating in Unit I and Unit II of Paks NPP. The operating VERONA system is not yet ready; there are some provisional solutions in the extrapolation of the readings of the self-powered detectors. The final system is due to be ready in the Summer of 1985.

The other significant work of the department is the dynamic modelling of nuclear power plants. In this period we finished the dynamic model of the primary circuit of Paks NPP and it was verified with measured transients. The development of a basic principle simulator for PWR plants has commenced.

The previously developed contact free primary flow-rate meter system is operating well as expected, at the first block of the Paks PWR. The same measuring system was installed at the second block of the power station, and the same work is in progress for the third block too. A fundamentally similar flow meter with sixteen channel correlation was developed for a GDR research institute, where it is used for velocity measurement of coal powder.

HEALTH PHYSICS

One of the main tasks in the Health Physics Department is the personal dosimetry, the routine operational radiation protection of the working places in the whole Research Centre and the continuous monitoring of the environment.

There have been further developments in the environmental monitoring system previously designed and constructed for the Paks Nuclear Power Station. After analysing the measurements of the first two years, a correlation technique has been introduced that decreases the minimum detectable dose rates below 1% of the natural background.

Results obtained in the fields of thermoluminescent and nuclear track dosimetry are also important. The whole body counter is equipped with a new computerized control and data evaluating system for determination of organ doses. New methods have been invented for the measurement of low activity samples.

Experimental and theoretical investigations are carried out for the construction of a stochastic lung model. This is intended to be used for the calculation of the deposition of aerosols inhaled into the human respiratory tract.

CHEMISTRY

In the last few years the research work of chemical and physical-chemical field has concentrated mainly on the water chemistry and corrosion properties of primary coolant for purposes of safe operation of the Paks Nuclear Power Plant, and on the investigation of a new energy source related to hydrogen energetics by photo-electrochemical methods. Analytical methods based on neutron activation analysis and mass spectrometry have been developed for the analysis of primary coolant, corrosion products, microelectronic materials and devices, as well as medical, biological, geological, agricultural and environmental samples. Basic research has continued in the fields of hot atom chemistry, the chemistry of organic astitine compounds, the structure of water and water solutions.

RESEARCH REACTOR

The WWR-SM research reactor has operated according to the schedule: 3360 and 3522 hours in the years 1983 and 1984, respectively. The reactor is to operate until the end of 1985, when it will be shut down for a reconstruction. The aim of the reconstruction is to change the main components and to raise the power to 20 MW. According to schedule, the reactor will be restarted in 1988.

INSTRUMENTATION FOR NUCLEAR PHYSICS AND TECHNIQUES

The Instrument System for Nuclear Industry - having been previously developed and containing about 60 modules - was completed by an analogue reactivity meter and a fast picoammeter. In cooperation with the IAEA a multichannel analyser with microcomputer intelligence was developed.

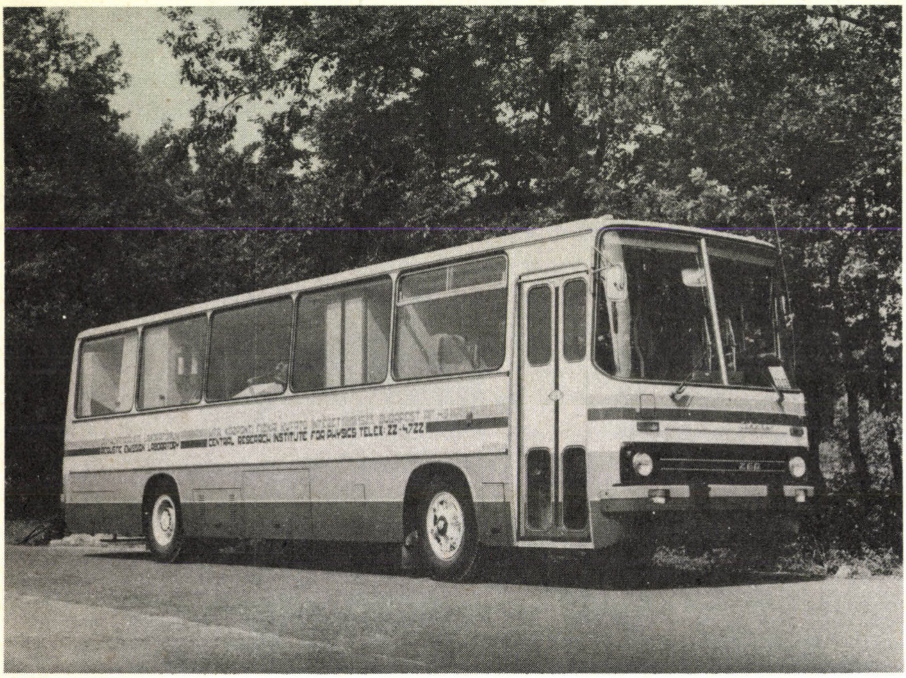

Fig. D-1

The 32 channel, computerized acoustic emission fault localizer and analyzer developed at KFKI is for testing the integrity of large structures like pressure vessels, long pipes etc. The instrument and necessary equipment are together are located in a bus produced also in Hungary.

Preparations were begun on the nuclear instrumentation system for the Institute's WWRS research reactor, which will be reconstructed in the next few years.

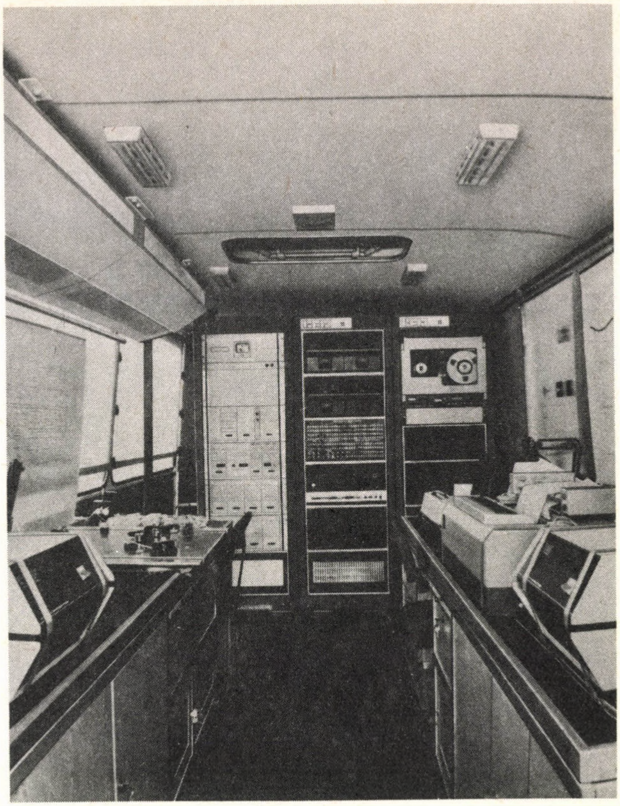

Fig. D-2
Inside view of the mobile acoustic emission laboratory

ACOUSTIC EMISSION TECHNIQUES

Acoustic emission as a modern, non-destructive testing technique will be more and more utilized in the nuclear industry. To promote the application of this method a mobile, computerized 32-channel acoustic emission laboratory for fault localization and analysis was developed and manufactured. Several measurements were accomplished in industrial settings. Besides this sophisticated laboratory a small, portable, battery operated four channel acoustic emission instrument, controlled by a microprocessor, was also developed, mainly for field applications (see *Figs. D-1,2,3*).

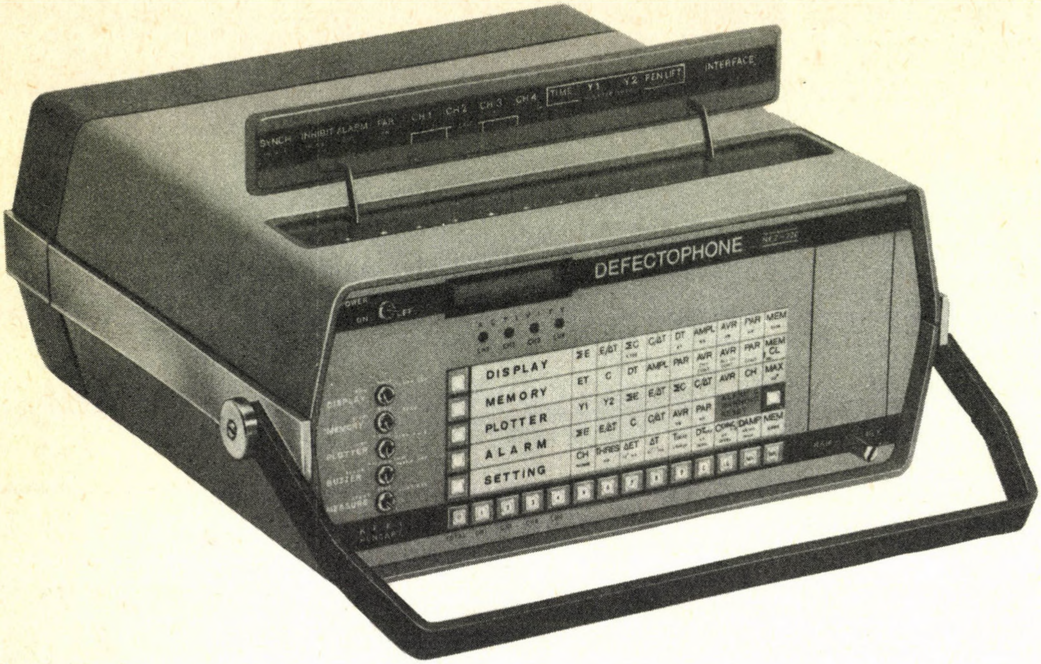

Fig. D-3

Microcomputerized, battery operated, portable four-channel acoustic emission instrument mainly for field usage

GROUP THEORY APPLIED IN REACTOR PHYSICS

M. Makai

It is well known how symmetry properties can advantageously be exploited in solving a linear equation. Reactor physics deals, among other things with determining the neutron distribution in a finite volume V. The neutron gas obeys either a linear Boltzmann (transport) equation (TE) or a linear diffusion equation (DE). The present work [1] is devoted to the application of geometrical symmetries of the finite volume V to boundary condition problems of the type

$$\hat{T}(\underline{x})\Psi(\underline{x}) = 0 \quad \underline{x}\in V, \tag{1.a}$$

$$\hat{B}(\underline{x})\Psi(\underline{x}) = f(\underline{x}) \quad \underline{x}\in \partial V, \tag{1.b}$$

where $\hat{T}(\underline{x})$ and $\hat{B}(\underline{x})$ are space dependent linear operators and $f(\underline{x})$ is a given function along the boundary ∂V. Furthermore $\hat{T}$ and $\hat{B}$ are such that if $\hat{P}$ is a symmetry of $\hat{T}$ it is also a symmetry of $\hat{B}$. For symplicity's sake only the face averaged boundary condition is considered in the present work.

In the linear Boltzmann equation the operators acting on the *angular flux* $\Psi(\underline{r},E,\underline{\Omega})$ are linear and the boundary condition fixes the value of a linear expression of the angular flux. The method to be presented has been developed in relation to neutron transport but is applicable to other linear transport problems as well. The symmetry properties of the transport and the diffusion equation are so similar that they may be treated in a unified way. The independent variables are denoted by $\underline{x}$ and they are the coordinates in the phase space, so $\underline{x} = (\underline{r},E,\underline{\Omega})$ in the transport problems and $\underline{x} = (\underline{r},E)$ in the diffusion problems. The energy dependence is considered in the context of the widely used energy group structure. The transport equation is written as

$$\underline{\Omega}\underline{\nabla}\Psi_g(\underline{r},\underline{\Omega}) + \Sigma(\underline{r},E)\Psi_g(\underline{r},\underline{\Omega}) = \sum_{g'} \int_{4\pi} d\underline{\Omega}'\Sigma(r;g',g,\underline{\Omega}\cdot\underline{\Omega}')\Psi_{g'}(\underline{r},\underline{\Omega}') . \tag{2}$$

In the diffusion problem the dependent variable is the scalar flux and the DE is

$$-D_g\nabla^2\Phi_g(\underline{r}) + \Sigma_g(\underline{r})\Phi_g(\underline{r}) = \sum_{g'=1}^{G} \left[\frac{\chi_g}{k_{eff}}\nu\Sigma_{fg'}(\underline{r}) + \Sigma_{g'\to g}(r)\right]\Phi_{g'}(\underline{r}) , \tag{3}$$

where the cross sections Σ have the usual meaning [2]. The physical process described by eq. (2) or by eq. (3) determines the cross-sections.

In neutron physics the *partial currents* are used as the boundary condition. Let $I_g^+(\underline{r})$ denote the *incoming current* and $I_g^-(\underline{r})$ the *outgoing current*, then

$$I_g^+(\underline{r}) = \int_{\underline{\Omega}\underline{n}>0} \Psi_g(\underline{r},\underline{\Omega})d\Omega , \tag{4}$$

and the similar expression for $I_g^-(\underline{r})$ is omitted. Throughout or analysis *the region V is assumed to be a regular body with n faces and the material distribution inside V is assumed not to break this symmetry.* The face averaged incoming currents are:

$$\partial V = \bigcup_{i=1}^{N} \partial V_i , \tag{5}$$

$$I_{gi}^+ = \frac{1}{F} \int_{\partial V_i} dF_i \int \Psi_g(\underline{r},\underline{\Omega})d\underline{\Omega} . \tag{6}$$

Both in transport theory and in diffusion theory the problem (2), (3) is often transformed to a so called response matrix form in which the outgoing currents are expressed as a linear combination of the incoming currents:

$$I^{-}_{gk} = \sum_{g'=1}^{G} \sum_{k'=1}^{N} T^{kk'}_{gg'} I^{+}_{g'k} \ . \tag{7}$$

Symmetry consideration can be utilized to diagonalize the response matrix of Eq. (7). As it is shown below, an advantageous separation can be achieved by using invariant boundary conditions, see Section 1. In a periodic lattice the solution is expressed as a linear combination of Bloch functions, see Section 2.

1. INVARIANT BOUNDARY CONDITIONS, RESPONSES

Let us condense the N values of $f(\underline{x})$ corresponding to the N faces of V (that we now call a cell) in vector $\underline{I} = (I_1, I_2, \ldots, I_N)$. Making use of standard technique of projecting out the irreducible components we obtain boundary conditions or incoming current patterns belonging to invariant subspaces. Such invariant incoming currents are given in *Fig. D-4* and *Fig. D-5*. Since the symmetry properties of the invariant subspaces of $f(\underline{x})$ coincide with those of the invariant subspaces of $\hat{T}\Psi(\underline{x})$ and $\hat{B}\Psi(\underline{x})$ as well, the operators $\hat{T}$ and $\hat{B}$ will be diagonal in the sense that $\hat{T}(\underline{x})$ or $\hat{B}(\underline{x})$ can not lead out from a given subspaces.

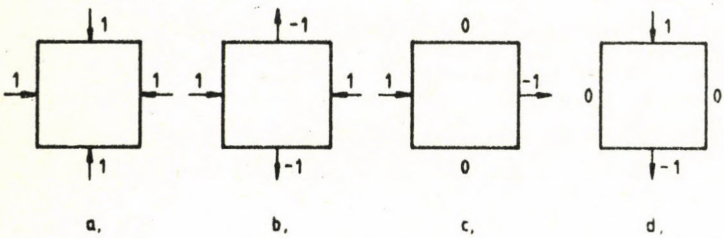

Fig. D-4

Invariant incoming current patterns in a square

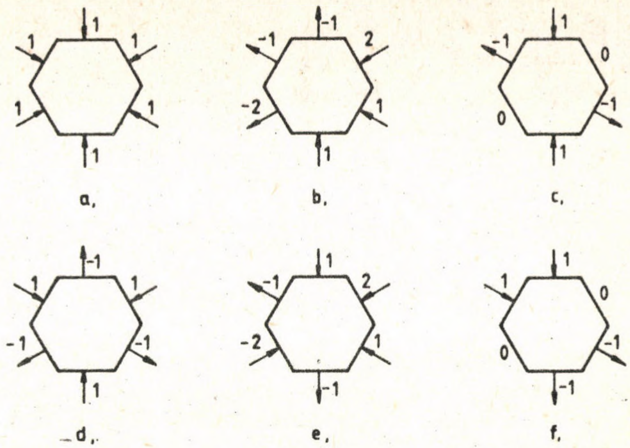

Fig. D-5
Invariant incoming current patterns in a hexagon

The invariant subspaces are used as follows. Let us decompose $f(\underline{x})$ as

$$f(\underline{x}) = \sum_{i=1}^{n_c} \sum_{k=1}^{\ell_i} c_k^{(i)} \cdot f_k^{(i)}(\underline{x}), \qquad \underline{x} \in \partial V \tag{8}$$

where n_c is the number of classes of the group of $\hat{T}$ and ℓ_i is the dimension of the i-th subspace. Since we have restricted ourselves to face averaged boundary conditions, the number of the independent $f_k^{(i)}$ functions is restricted to the number of faces. In such cases some of $f_k^{(i)}$ will be zero. Let us solve the problem

$$\hat{T}\Psi_k^{(i)}(\underline{x}) = 0, \qquad \underline{x} \in V \tag{9a}$$

$$\hat{B}\Psi_k^{(i)}(x) = f_k^{(i)}(\underline{x}) \qquad \underline{x} \in \partial V. \tag{9b}$$

Now the solution of problem (1) is given as

$$\Psi(x) = \sum_{i=1}^{n_c} \sum_{k=1}^{\ell_i} c_k^{(i)} \Psi_k^{(i)}(\underline{x}) \tag{10}$$

$\Psi_k^{(i)}(\underline{x})$ is called a response, as we can give a well determined physical meaning to every invariant incoming current pattern. In a square cell, see *Fig. D-4*, they represent a homogeneous environment (a,, an environment with gradients (c, and d,), and a more complex environment (d,) and the corresponding $\Psi_k^{(i)}$ specifies how the cell behaves in the given environment.

In a region composed of a large number of cells, the solution is often determined by iteration: we sweep through the cells until two consecutive solutions are close enough together. In such methods the responses do not depend on the actual positions of the cells; moreover, the coefficients $c_k^{(i)}$ are obtained from a finite difference-like scheme.

2. PERIODIC LATTICE

The case when V has a periodical inner structure is of great importance since most of real reactor cores contain such volumes. That particular case shows extraordinary similarity to certain problems of solid state physics. If V is infinite, the eigenfunctions of $\hat{T}$ are Bloch functions:

$$f_{\underline{B}}(\underline{r},E,\underline{\Omega}) = e^{i\underline{B}\underline{r}} u_{\underline{B}}(\underline{r},E,\underline{\Omega}) , \tag{11}$$

In the Bloch function basis both $\hat{T}$ and the reaction rate forming operators in the TE will be diagonal. Without going into details, the solution belonging to the largest eigenvalue is given as

$$\begin{aligned}\Psi(r,E,\underline{\Omega}) &= \int_{R_o} w(\underline{B}) f_{\underline{B}}(r,E,\underline{\Omega}) d\underline{B} \\ &= \phi_M(\underline{r}) u_o(r,E,\underline{\Omega}) + \sum_j \frac{\partial}{\partial x_j} \phi_M(r) u_{1j}(\underline{r},E,\underline{\Omega}) \\ &= \sum_j \frac{\partial^2}{\partial x_j^2} \phi_M(\underline{r}) \cdot u_{2j}(r,E,\underline{\Omega}) + \ldots ,\end{aligned} \tag{12}$$

where

$$\phi_M(\underline{r}) = \int_{R_o} w(\underline{B}) \exp(i\underline{B}\underline{r}) d\underline{B}' , \tag{13}$$

and

$$u_B(r,E,\underline{\Omega}) = u_o(\underline{r},E,\underline{\Omega}) + \sum_j iB_j u_{1j}(r,E,\underline{\Omega}) + \ldots . \tag{14}$$

The set R_o contains all the admissible $\underline{B}$ vectors and is determined by geometry on the one hand (geometrical buckling) through the boundary condition prescribed on ∂V, and by material distribution (material buckling) on the other hand through the neutron balance.

As we see, the solution (i.e. the neutron distribution in the phase space) is composed of functions of two kinds. The macroflux $\phi_M(\underline{r})$ describes the global neutron distribution in V, while the periodic u_i functions reflect mostly the internal cell structure.

When considering only face averaged boundary conditions, we can realize a correspondence between the components of $u_{\underline{B}}$ in eq. (14) and the boundary condition patterns in *Fig. D-4*. As u_o is the solution of the TE in an infinite lattice, it corresponds to structure a, u_{1x} is the response of the cell to an x directed current so it corresponds to structure c, and so on. Making use of this correspondence the formula (12) giving the neutron distribution can be generalized [3] to cases when the cells are different, e.g. they contain control rods, fuel rods or structural elements.

In this rather general case the macroflux is obtained from a finite difference form of the DE, irrespectively of the cell being treated in transport or diffusion approximation [3,4].

3. AN ANALYTICAL COARSE MESH METHOD [5]

The coarse mesh (CM) method is a numerical tool of solving the DE in a volume consisting of large, homogeneous regions called nodes. Below, an analytical CM method is outlined, which is based on the considerations of Sect. 1. Now the responses have a closed form and we get the response matrices after a simple calculation.

The solution of the DE is composed of eigenfunctions of the Laplace operator. The eigenvalues α_k^2 of the DE can be found from the following eigenvalue problem:

$$(-D_g\alpha_k^2 + \Sigma_g)t_{kg} = \sum_{g'=1}^{G} \left(\frac{\chi_g}{k_{eff}} \nu\Sigma_{fg'} + \Sigma_{g'\to g}\right)t_{kg'} \,, \qquad (15)$$

$$k = 1,\ldots,g; g' = 1,\ldots,G \,.$$

From the eigenvalues α_k^2 and the eigenvectors $\underline{t}_k$ an analytical solution is formed as

$$\Psi_g(\underline{r}) = \sum_{k=1}^{G} \int_{|\underline{B}|=1} C_k(\underline{B})\exp(\alpha_k\underline{B}\underline{r})t_{kg}\, d\underline{B} \,. \qquad (16)$$

Let us assume

$$C_k(\underline{B}) = \delta(\underline{B} - \underline{B}_k)\cdot C_i^{(k)} \,. \qquad (17)$$

Then the irreducible components of $\Psi_g(\underline{r})$ are linear combinations of exponential functions. Let $S_{ig}^{(k)}$ denote the i-th irreducible component associated with the k-th eigenvalue. The flux $\Psi_g(\underline{r})$ is now

$$\Psi_g(\underline{r}) = \sum_i \sum_{k=1}^{G} C_i^{(k)} S_{ig}^{(k)}(\underline{r}) \,, \qquad (18)$$

where the subscript i runs over the bases of the irreducible subspaces. In CM methods the incoming currents are given on the boundary of the node.

Let us i-th irreducible incoming current patterns (see *Figs. D-4* and *D-5*) be $\underline{e}_i$. Then

$$\underline{I}_g = \sum_i m_{ig} \underline{e}_i \quad . \tag{19}$$

From the condition that the incoming current of the corresponding analytical solution should equal m_{ig} we have equations for $c_i^{(k)}$:

$$\sum_{k=1}^{G} c_i^{(k)} \hat{B}[S_{ig}^{(k)}(\underline{r})] = m_{ig} \; , \qquad g = 1,\dots,G; \quad i = 1,\dots,n_c . \tag{20}$$

As the irreducible subspaces are linearly independent, the above set of equations disintegrates into n_c independent sets. With known $c_i^{(k)}$ whe have a complete analytical solution in the given node. An iterative procedure is established as follows. We sweep through the nodes, carrying out the following steps:

a) collect the incoming current of the given node;
b) determine the analytical solution from the $S_{ig}^{(k)}$ functions;
c) obtain the outcurrents from the analytical solution;
d) take the next node;
e) repeat the above steps until convergence has been reached.

In passing from one node to another continuity ensures that the outcurrent is the incurrent of the adjacent node.

Table 1

Results for the GA9A1 Benchmark Problem

Code	k_{eff}	Point/Node	ΔP (%)	Δϕ	Time[a] (s)	Computer	Laboratory
BUG 180	1.11815	48	0.0	10^{-5}	9660	UNIVAC 1108	
GRIMHX	1.12028	6	5.1	10^{-5}	26	IBM S-370/195	]GA, USA
GRIMHX	1.11863	6	3.1	10^{-5}	10	IMB S-370/195	
VENTURE	1.11860	54	-	10^{-5}	172	IBM 360/195	]ORNL, USA
VENTURE	1.12725	1	-	10^{-5}	37	IBM 360/195	
DIFGEN	1.11640	--	4.8	10^{-5}	36	CYBER 174	]IKE, FRG
DIFGEN	1.11690	--	6.0	10^{-5}	230	CYBER 174	
VALE	1.11814	48	-	10^{-5}	154	IBM 360/91	]ORNL, USA
VALE	1.11671	43	-	10^{-5}	18	IBM 360/91	
SIXTUS[b]	1.11650	1	2.4	$5x10^{-5}$	97	EC-1040	]EIR, Switzerland
HEXAN	1.11888	1	1.5	$3x10^{-5}$	537	EC-1040	]KFKI, Hungary

[a] *1 s IMB 360/195 = 2 s IBM 360/91 = 4 s CYBER 174 = 11 UNIVAC 1108 = 30 s EC-1040.*

[b] *EC-1040 adapted version.*

The above described procedure has been implemented in computer programs. Above, test results obtained by HEXAN are compared to other results. In *Table 1* the effective multiplication eigenvalue k_{eff} and the maximum error in the power distribution (ΔP) are compared. The problem represents a high temperature gas cooled reactor core. From the results it is apparent that HEXAN has not yet been adequately equipped with accelerating tricks but the analytical solution has proved superior to the traditional polynomial methods [6].

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A NEW MEASURING INSTRUMENT OF THE MICROCOMPUTER AGE: DEFECTOPHONE

J. Geréb, G. Kruchió, B. Lafranco, P. Pellionisz

Abstract A new measuring instrument has recently been developed in KFKI for the measurement of acoustic emission waves originated from solid materials under mechanical stress. The small, portable, battery- and mains-operated device takes advantage of the general availability of microcomputers. The internal microprocessor oversees its operation and controls the measurements. In addition, the data processing tasks can be transferred to computers (even simple p.c.-s can be applied).

The paper summarizes the fundamentals of the acoustic emission measurement technique and describes the main philosophy of the device. Details are given on such unique features as array-type programming on the front panel, replaceable memory module, self-checking, etc.

1. INTRODUCTION

The deformation of materials and structures may result emission of micro-level acoustic waves in the frequency range from audible up to several MHz. The acoustic emission (a.e.) waves are converted into electric signals by using piezoelectric transducers mounted on the surface of the object under investigation.

Even the analysis of signals from one single transducer can yield a great deal of information about the condition of the tested material (metals, rocks, composites, etc.). Typical emission parameters are presented in *Fig. D-6* (BURST). Similarly, by sampling continuous acoustic signals, failure indications can be obtained in early phase (e.g. leakage) - as *Fig. D-6* shows (CONT).

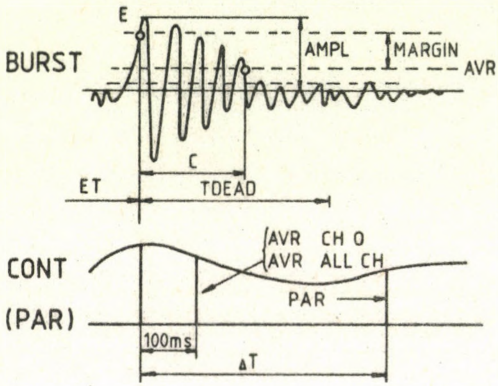

Fig. D-6

Measured parameters of an a.e. signal burst and of continuous acoustic or parameter signals

If sensors are placed at different points of the tested structure, additional important information can also be obtained. Since an acoustic emission burst takes different times to reach the individual sensors at different distances from the source the measurement of these delays makes possible source location calculations.

Modern a.e. measuring devices measure many a.e. signal and time parameters for each event. These instruments can be divided into two groups according to information processing. Devices in the first group only display and plot actual data - they are relatively simple, small and not very intelligent. A typical device in the second group has a built-in CRT graphic display, an internal data-processing computer with a number of software-items and hardware peripherals, not to mention the measuring circuits for at least 4 a.e. channels.

Our new device, the DEFECTOPHONE NEZ-220 incorporates a new philosophy: it is an instrument that records data from the stream of acoustic waves, gives a local display, incorporates a plotter, has alarm and validity check possibilities for 4 channels, and either makes data available to any computer for on-line processing or stores them in its replaceable memory module for later use. It is a small and simple device, yet powerful and variable - taking advantage of the fact that personal computers are almost as common and accessible in today's laboratories as telephones.

2. THE MEASURING TASK

The instrument - named DEFECTOPHONE NEZ-220 - should be applied in a.e. measurements either in research laboratories or in industrial and field applications. The device is intended for the international instrument market, therefore it should contain all the accessories of four-channel measurements: a set of acoustical sensors and amplifiers. The latters have logarithmic amplitude characteristics, since a.e. activity has a very high and unpredictable dynamic amplitude range.

The main unit - the measuring device itself - is portable, rugged and battery operated. It conforms field requirements and is user friendly. In laboratories, it can be operated also from the electrical mains by connecting its mains power pack.

The device has four a.e. input channels and another one for registrating a technological parameter, like force, pressure, temperature. With DEFECTOPHONE, both continuous and burst-like acoustic signals can be identified. On burst type emission signals only that one is completely identified which appears first among the four detectors. On this signal amplitude, time, count, and rate measurements are done each time when the signal crosses a threshold which is automatically adjusted to the background noise.

The signals following the first one in a burst are measured only in the time domain: delay times and detector codes are registrated at each event.

In *Table 1* the parameters measured by the DEFECTOPHONE NEZ-220 are presented:

Table 1

Measured parameters by the Defectophone

Parameter		*Range*	*Resolution*	*Display*	*Storage*	*Plotter*	*Alarm*
* *Event elapsed time,*	*ET*	*0...655,350 s*	*1 ms..10 s*		+		
* *Events total,*	*ΣE*	$0...10^8$	*1*	+		+	+
* *Events rate,*	*E/ΔT*	$0...10^8$	*1*	+		+	+
* *Counts/event,*	*C*	$0...10^6$	*1*		+		+
* *Counts total,*	*ΣC*	$0...10^8$	*1*	+		+	
* *Count rate*	*C/ΔT*	$0...10^8$	*1*	+		+	+
* *Peak amplitude,*	*AMPL*	*0...127 dB*	*1 dB*	+	+		
□ *Delay time (geotechn.),*	*DT*	*0..40,950 µs*	*10 µs*	+	+		
□ *Delay time (metallurgy),*	*DT*	*0...4095 µs*	*1 µs*	+	+		
□ *Average,*	*AVR*	*0... 127 dB*	*1 dB*	+	+	+	+
Technological param.	*PAR*	*0... 2,5 V*	*10 mV*	+	+	+	+

**For the first channel* □ *For all channels* *ΔT = 100 ms, 1 s, 10 s, 100 s.*

Not only measurement, but alarm, recording and a.e. data acquisition tasks can be performed with the same device. Different Eurocard-type plug-in units can be placed in its front panel slot. The first one, the NEZ-220-51, serves as an 18 K-byte memory for storing measurement data. It can be read by any computer using RS-232 serial interface. The filled module can also be exchanged for a new one if it cannot be read under field conditions. Measurement data can be sent out to be analysed, displayed or listed by computers, or to be recorded by simple plotters. Several Defectophones can be synchronized and operated by using one as a master and the others as slaves, in order to realize systems with a large number of a.e. channels.

3. MAIN FEATURES OF THE DEFECTOPHONE

The instrument is controlled by a Z-80 microprocessor supported by a 10 K byte machine code program. The built-in intelligence provides a number of highly useful capabilities for the device. The software carries out so many tasks that the hardware can be simple, its main function being the digitalisation of the acoustic emission parameters.

The software contains interrupt service routines. There are five procedures which can cause interrupt: the time measuring and sampling procedure, the delay time invalidation, the changing of switches or push-buttons, the loading of transmitter buffer register and the valid burst type event. Some software routines control the front-panel. They determine the actual value of any acoustic emission parameters that can be seen on the display, and control the LED's in accord with the content of the output ports.

It is possible to change the parameters of the measurement from the front-panel. The instrument has a write-in-a-number state, which allows one to give a new value to the parameter by push-buttons on the front-panel. There is an LED in each push-button. The LED lights, does not light or flashes, depending on the function of the push-button and the state of the instrument. If a button is pushed, one of the interrupt routines will be activated. This routine controls the LED-s and the display in accord with the contents of the ports.

Thus the microporcessor makes possible the numerical programming by means of the push-buttons on the front panel.

If the programming on the front-panel is not correct, the instrument alerts the user and corrects the error if it is possible. If a new value is too big or too little, the instrument does not change the parameter and the buzzer sounds. If the instrument has to round off a new value, the instrument does it and gives a short whistle. If there is a controversial step in programming, the instrument signals by a short whistle.

The instrument checks itself. It checks the voltage of the batteries when the instrument starts measuring and at 100 minutes intervals, and it tests the operative memory at power on.

If the self-checking results in an error condition, a failure code can be seen on the display and the buzzer starts working. The instrument checks the validity of the measurments. An event is rejected if validity criteria are not met by the input signals. The validity checking is carried out both by software and hardware.

The instrument has an interchangeable memory module and a RS-232 serial computer interface for on-line and off-line analysis. The memory module stores the actual setting of the instrument and the measured data. The stored information is preserved for about 3 months. If there is a memory module in the plug-in space of the central unit, the instrument will set itself automatically to a preset state following the power-up, without any programming intervention. Thus the instrument is able to set a previous preset state quickly and simply.

The information to be stored is not only written into a memory module but can be sent also to a computer via an RS-232 serial interface. The computer can be almost any simple personal computer (Sinclair Spectrum, Commodore C-64, etc.), since most of them are equipped with such a data communication interface. Thus on-line data analysis is possible by the computer. The content of the memory module can be analysed off-line, too. The instrument can read the memory module and send the data to the interface.

Instead of the memory module other units can be operated in the plug-in space. A service module will be developed. This module disables the microprocessor and tests all the hardware.

4. DEFECTOPHONE - AN INSTRUMENT SUPPORTED BY PC-s

Instead of limiting the performance of the instrument by a fixed set of simple data processing programs built into the device, a flexible interface has been developed. Measured data can be read from the memory module through the RS-232 serial interface immediately or after having been stored in the memory module. The basic configuration of the instrument contains a 18 K RAM memory module. A larger capacity module will be developed later.

The data structure used in the memory module is the following. The first 45 bytes store the instrument setting, the rest stores the measured data. The data consist of blocks. There are three different types of blocks: comment blocks, event blocks and sample blocks. Comment blocks will be written automatically into the memory at the beginning of each measurement and at changes in instrument setting. Event blocks contain the selected parameters of the acoustic emission signals. Sample blocks contain the selected parameters of continuous signals. The transfer rate can be set in the instrument by switches in accordance with the setting of the computer. The selectable rates are the following: 150, 300, 600, 1200, 2400, 4800, 9600, 19200 Baud. It takes about 12 minutes to read the 18 K byte memory module at 300 Baud, while about 12 sec at 19200 Baud.

Through the RS-232 interface, a computer can receive the stored data for analysis, and output results on a CRT display or make hardcopy. The computer programs are developed by the manufacturer or by the users. These programs may be written in high level computer language: BASIC, FORTRAN, etc. The developing group made such programs for COMMODORE C-64, the most common personal computer in Hungary. The program consists of two parts. The first part is the date-capture-part. This part is an interrupt routine. Each received bit causes an interrupt on the C-64, so the transfer rate can not be too high: the speed of the data transmission is at most 1200 Baud. This feature of the C-64 limits the on-line analysis but does not limit the off-line analysis. The interrupt routine writes the received data to a floppy disc. This part is a machine code routine because of the speed requirements.

The second part of the C-64 routine is the data processing program. This program selects the data stored onto the floppy disk and displays the requested functions (for example: $\Sigma E(t)$, $\Sigma C(p)$, etc.) on the CRT display or plotter. The program has arithmetic tasks: producing cumulative parameters (ΣC, etc.), and two-dimensional source location. The location calculation can be performed on-line. The source location process requires a fixed geometry transducer-array.

The most universal array consists of four detectors put to the vertices and the middle of a regular triangle.

5. INSTRUMENT CONSTRUCTION

Because of the portability and the battery operation, the instrument was designed for low power requirement. For this reason CMOS integrated circuits were chosen for digital circuits and static RAM-s. The central unit can be supplied either by a mains pack or by a battery pack. The battery pack operates for a maximum of 13 hours without charging. The power requirements for the main unit: 4,6,..., 5,4 V/1,2 A and for the amplifiers: 10 ... 13 V/40 mA.

In addition to the Z-80 CPU the device has other two system elements: a Z-80 SIO and Z-80 CTC. These two system elements realise the interrupt structure and control the interface. The main features of the Z-80 CPU (2 MHz clock frequency, 8 bit data bus, 64 K byte direct addressable memory) are suitable for the requirements of this instrument.

The electronics is built on six cards. About half of the electrical components are made by socialist countries.

The main unit has portable construction. The dimensions of the main unit: 145x337x260 mm, the batteries pack: 145x337x57 mm, the mains pack: 145x337x73 mm. Weight of the main unit: 8 kg, the batteries pack: 4 kg, the mains pack: 2,5 kg.

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RESEARCH INSTITUTE FOR MEASUREMENT AND COMPUTING TECHNIQUES (MSZKI)

The Research Institute for Measurement and Computer Techniques supplies the research centre with minicomputer systems clustered around the mainframe computer and in the measuring centres. This provides the computer base for the experimental and theoretical work of scientists in the research centre.

Our institute has also established a good reputation as a computer supplier for OEM companies and as an application systems house. We provide complete solutions in industrial and laboratory process control, business data management and scientific computations applications.

We have a small production line where, in cooperation with a number of external partners, our design methods can be tested in small series manufacturing. Another way of having a feedback from manufacturing is to supply the industry with our licences. In both ways, we feel, we are contributing to raising the level of computer-technical culture of Hungary.

HARDWARE DEVELOPMENT

Of the research and development activities of this department in the last two years, the efforts aiming at a system exploring the Halley's comet must be first mentioned. Applying the techniques of the fields of image processing and microprocessing, not only was the system completed but important knowledge and techniques have been learnt that can be widely used in the future.

During these past two years the development of the TPA-11/440 megamini computer system has been completed and production in small series has been started. This computer has a new architecture and applies new technology, providing a base for computer applications in KFKI during the second half of this decade. As an example of such applications, blocks III and IV of the atomic reactor in Paks will be controlled by a dual TPA-11/440 system.

The development of local networks has been considered as urgent. A local network called LOCHNESS was developed, and the experts of Computer Department made important contributions to the hardware development. One of its first applications will be a Tokamak data acquisition system.

In the field of professional personal computers, two computing tools must be mentioned: the TPA Quadro which is compatible with the TPA-8 family of minicomputers, and the TPA Janus which has two faces, one compatible with the TPA-11 family, and the other with the CP/M operating system.

SOFTWARE DEVELOPMENT

We have designed and implemented a 1 Mbit/s local area network called LOCHNESS (LOCal High-speed NEtwork SyStem) dedicated for process control applications. The line access control enables station and message priority. First installations using TPA 11/48 minicomputers and ICC (Intelligent CAMAC Crate controller) microprocessors will begin in 1985.

Based on this local area network we developed a distributed version of the PCDB (Process Control Data Base) system. The pilot project is the T-15 Tokamak experiment control and data acquisition system. The man-machine interface is realised by the DICOM (Display Communication) program package. This package helps the operator to display the data stored in the PCDB data base using alphanumeric or graphic displays and touch panels.

We have implemented an experimental Ada compiler on a PDP-11 compatible machine but its performance does not satisfy any commercial requirements;

it uses too much time and needs too much memory. Owing to the features and capabilities of Ada language, we have proved, it is not appropriate for 16-bit architectures.

In computer graphics we implemented packages for business graphic and engineering applications. We are now designing an interactive graphic editor and a printed circuit documentation system.

A CODASYL data base application is on the way which will support our institute's administration.

In the protocol research we finished the PROMIN I. protocol modelling package and took part in a protocol testing project for SWIFT (Society for Worldwide Interbank Financial Telecommunications).

As a good example of international cooperation we took part in the Giotto project (FRG) based on our experience in the VEGA (Venus-Halley comet) space research project. We also contributed to the development of an automatic warehousing system for Philips in Eindhoven, Holland.

We finished the implementation of a word processing system for the TPA-8 minicomputer family, a Personal Information Management System (PIMS), a spreadsheet-like calculator program named SCC (SCreen-oriented Calculator) and an integrated circuit tester system for the TPA-11 family. We began the installation of wide area networks and preparations for the institute's local area network are on the way.

LABORATORY APPLICATIONS

CAMAC SYSTEM

The development and final testing of the multiplexer/demultiplexer module family have been completed. A memory module with the maximum capacity the Intelligent Crate Controller can handle, a CAMAC modem, a modified time base generator, and a PROM programmer have been designed. The testing of a CAMAC module that interfaces the LOCHNESS local network has been continued.

LONG-RANGE REAL-TIME SYSTEM

As a start towards the construction of a new real-time system, based on international standards and replacing the existing CAMAC, an experimental system was built in Euro mechanics. This EURO-86 system contains several processors, memories, peripheral interfaces and a power supply. The system will be expanded in 1985 but the final version will be delayed until the standards have been stabilized.

ICA-80 MULTICHANNEL ANALYZER

A new expansion unit has been designed for the programmable multichannel analyzer ICA-80 which contains two floppy disks and twelve empty CAMAC stations where special modules, eg. high-voltage power supply, amplifier or coincidence unit, can be inserted.

APPLICATIONS

- a final testing device, containing an Intelligent Crate Controller, has been installed at Tungsram Co. for collecting data from 100 measuring stations of high-power gas-charged light source manufacturing lines.

- a gate array testing device was delivered to the Microelectronics Company in cooperation with other institutes.

- an astronomic measuring system was installed at the observatory of Burakan in the Soviet Union.

- the design and verification of data acquisition and control systems for Tokamak applications have been continued.

- an intelligent subsystem has been designed for MALEV which interrogates aeroplane black boxes.

BUSINESS DATA PROCESSING APPLICATIONS

During the past two years, we concentrated on putting on-line transaction systems into our business data processing applications. These systems provide real-time data entry and processing facilities and supply information for working places in the office. Data processing is controlled by the actual working process in a way that, in the execution of all the working phases, the employees use their on-desk terminals and store transaction data, together with their consequences, immediately in a data base. Decisions and transactions are being made using "real-time" information from this data base.

The application potential of this task solution technique is rather wide: it can be effectively used in stock and production control, banking and trading processes, and in place reservation systems.

MINICOMPUTER APPLICATIONS

The main task of this department, created in 1984, is the development of such application systems that aim at complex production control, utilizing the experiences gathered by the institute in the fields of business data management and process control. This aim will be expanded later to include automatic production systems.

The development of a workshop production control system with limited features was begun. It is an integrated system based upon a professional personal computer as the central unit and workshop terminals with microprocessors. The system will be capable of the supervision, administration and control of a mechanical workshop with 100-200 machines.

The department directed the development of the National Telemechanical System which is based upon a computer network supervising and controlling the operation of gas pipelines in Hungary. The system was installed in the summer of 1984, and now the business data management system of the Gas and Oil Transport Company is being developed with the aim of integrating the two systems in the future.

TPA-11/440 MEGAMINI COMPUTER

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The TPA-11/440, with the highest performance in the TPA family, has been designed with an architecture suitable for a wide range of applications.

The TPA-11/440 is entirely upward instruction-compatible with the existing TPA-11 and SM computers. UBUS-compatible peripherals can, of course, be connected to the TPA-11/440, so the peripheral interfaces already developed for the TPA-11 family can be used in TPA-11/440 systems as well.

Because of the rapid spread of cheap and sophisticated LSI and MSI integrated circuits, it was possible to respond to increasing user requirements and design the TPA-11/440 to provide users with an unusually *great number of standard functions*. This kind of design philosophy ensures both better cost/performance ratios and highly reliable operation.

STANDARD FEATURES OF TPA-11/440

- three processor modes: kernel, supervisor, user;
- separate instruction and data space;
- four new control instructions (MFPD, MTPD, SPL, CSM);
- 46 new floating-point arithmetic instructions (FP11);
- memory segmentation and multi-user protection;
- 16K byte cache memory;
- 32-bit wide internal synchronous bus with throughput of 8M byte/sec for higher I/O potential;
- 0.5M byte operative memory with error correction code (ECC);
- 22-bit mapping of UBUS addresses;
- intelligent ASCII console;
- self-diagnostics;
- two separate serial asynchronous lines for connection of terminals, or backup peripherals;
- bootstrap loader.

OPTIONS

- 52 new, character-string and decimal arithmetic instructions (CIS);
- max. 4M byte operative memory in increments of 0.5M byte;
- battery backup;
- defining of special, new instructions through user microprogramming.

INSTRUCTION SET

Beyond the familiar instruction set of the TPA-11 and SM4 computers the TPA-11/440 offers *46 new standard floating-point instructions* which make its numeric data manipulation much more effective. With the TPA-11/440 we can now support application areas, poorly supported so far, such as scientific-engineering measurements, interactive graphics and laboratory, industrial, medical real-time, computation-intensive process control.

The availability of the newly introduced floating-point instructions enables the users of the TPA-11/440 to employ the *FORTRAN IV PLUS* compiler, enhanced version of FORTRAN IV. The FORTRAN IV PLUS is extremely useful in scientific and engineering environment.

The floating-point instruction subset has the following main characteristics:

- single (32-bit) and double (64-bit) precision mode;
- 8-digit accuracy in 32-bit mode, 17-digit accuracy in 64-bit mode;
- flexible addressing modes, six floating-point registers with length of 64 bits each;
- arithmetic error handling.

The BASIC and APL programming languages can also make good use of the floating-point instructions available in TPA-11/440 systems.

A modern minicomputer should also have a potential in the field of data-intensive applications as well. For the first time in the TPA-11 family, the TPA-11/440 offers *52 new, special data handling instructions*, optionally, through microcode extension in a very cost-effective way.

The commercial instruction set (CIS) involves the following functions:

- decimal arithmetic;
- character-string handling;
- data format conversion.

The use of the optional commercial instructions in TPA-11/440 systems is especially effective when the *COBOL compiler* is used.

ARCHITECTURE

During design of the genuine TPA-11/440 architecture there were two basic considerations:

- TPA-11/440 should meet user requirements in the 80's; and
- TPA-11/440 architecture and input/output potential should serve as basis for development of devices with 32-bit instructions and 32-bit virtual addresses.

It is for this reason that a 32-bit wide internal bus, - X b u s - , is used as the main data path of the TPA-11/440 system architecture. The throughput of Xbus is 8 Mbyte/sec on the average, 4-5 times higher than that of UBUS.

Main characteristics of Xbus:

- data width: 32 bits;
- maximum directly addressable memory range: 16M byte/24 bits (only 4M byte is used in TPA-11/440);
- synchronous control with 125 nsec cycle time;
- distributed arbitration;
- potentially suitable for multi-processor environment;
- 32 bits read/500 nsec - 8 Mbyte/sec;
- 32 bits write/250 nsec - 16 Mbyte/sec;
- number of program interrupt levels: 4;
- number of devices on Xbus: 16;
- Xbus latency: min. zero, max. 125 nsec if other request is not in progress.

In the TPA-11/440 system architecture the components performing at a higher data rate are connected to Xbus *(Fig. E-1)*:

- memory modules with the capacity of 0.5M byte each;
- central processor through the cache memory;
- UBUS adapter realizing UBUS - Xbus protocol conversion and UBUS - memory address mapping;
- mass storage controllers with high data rate;
- special function processors;
- Z80 microprocessor based console and diagnostic subsystem, for easier availability purposes.

The 16K byte standard cache memory decreases the average main memory access time, so increases system throughput. Memory modules with 0.5M byte capacity each can be interleaved for higher input/output

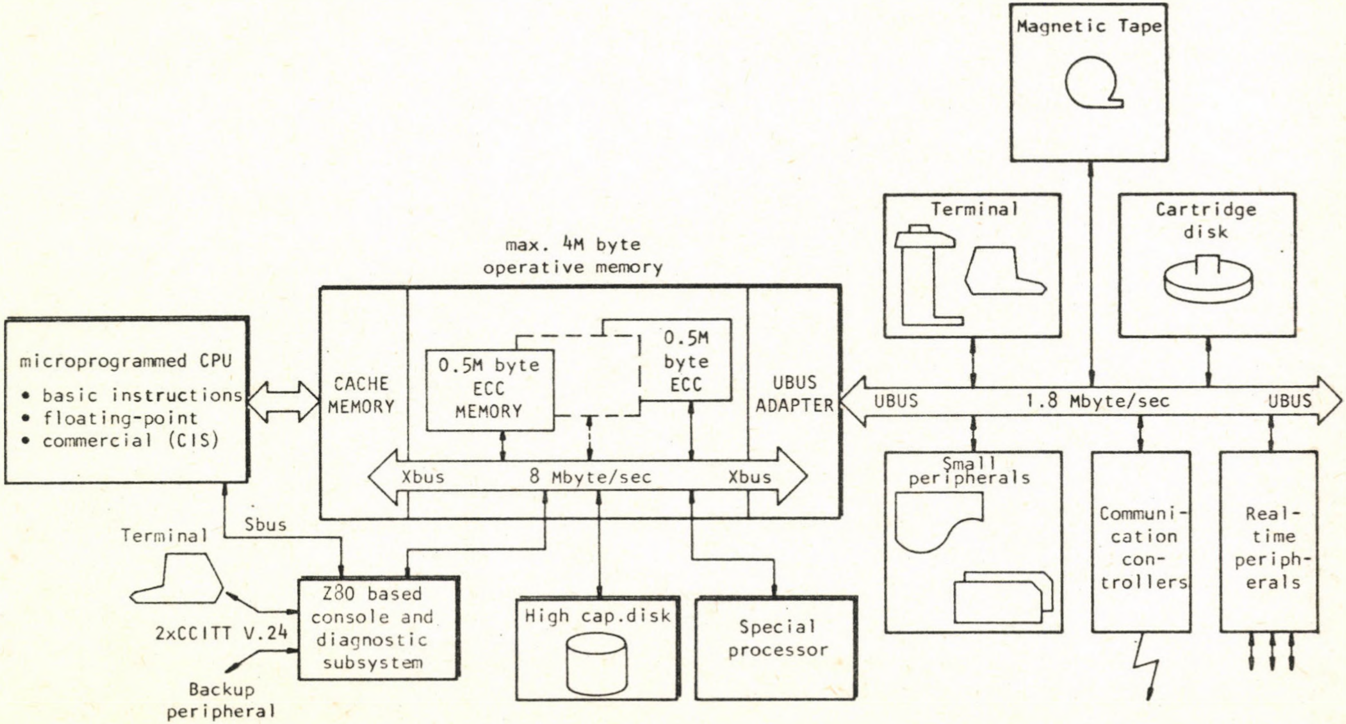

Fig. E-1

TPA-11/440 System Architecture

potential. Each memory module uses 32+7 bits data format where 7 bits serve to automatically correct any one-bit error in a 32-bit double-word. The standard use of the error correction code provides extremely high reliability in memory transfer.

IMPLEMENTATION

The TPA-11/440 electronics is realized in the System Unit (SU) structure already familiar with other TPA-11 models. The basic central processor system configuration, including 0.5M byte ECC memory, is implemented on eight printed circuit boards. 64K bit dynamic MOS memory chips are used in the memory. The central processor is based upon the AM 2900 bitslice family. The cache memory uses high-speed static RAMs.

SOFTWARE

The TPA-11/440 is entirely upward compatible with the earlier introduced members of TPA-11 family, and with the SM4 computer, respectively. For making use of the features offered by the TPA-11/440 systems, the RSX-11M, RSX-11M PLUS and UNIX operating systems are recommended.

APPLICATION

A number of TPA-11/440 systems have been operating in various fields of application such as scientific measurements, engineering design, medical research, industrial process control and data base management. A TPA-11/440 configuration equipped with 2M byte operative memory and a few hundreds of megabyte disk capacity is shown in *Fig. E-2*. It was installed at MASPED, Budapest, and is used for database management and software development.

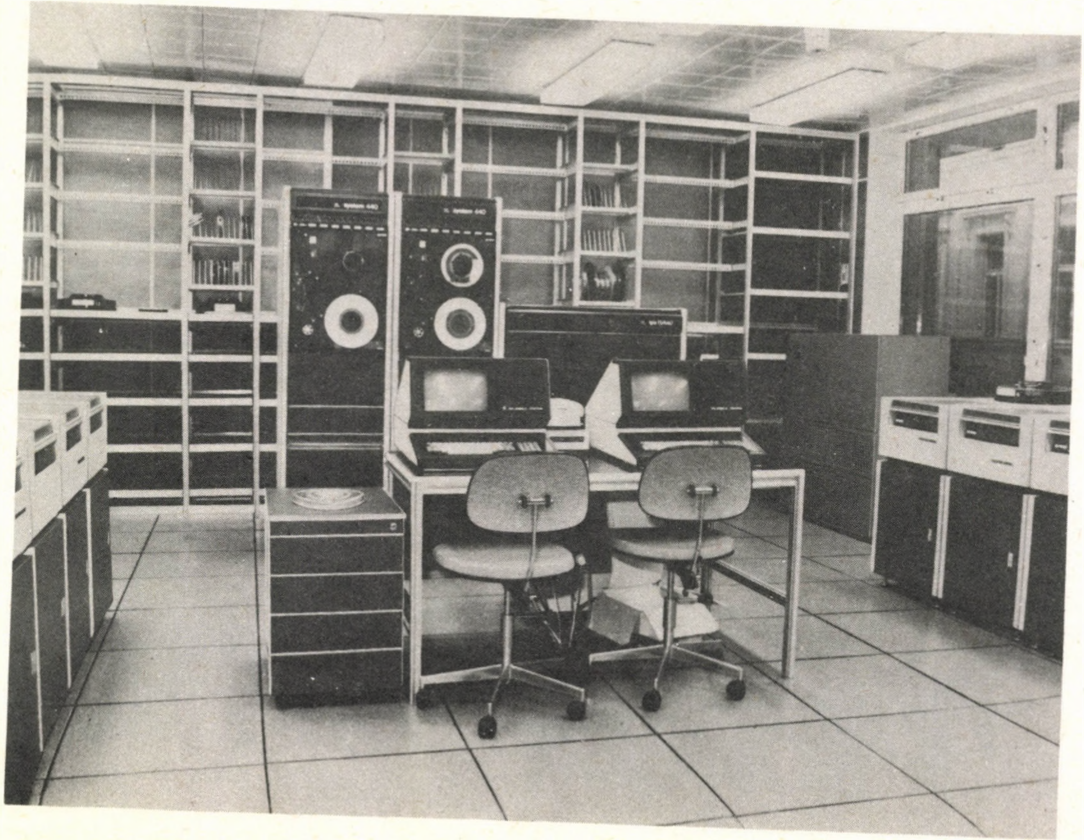

Fig. E-2

TPA-11/440 System at MASPED

LOCHNESS, A LOCAL AREA NETWORK

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INTRODUCTION

A local area network has been developed with laboratory automation and process control as the primary fields of application. The architecture of the local area network takes into consideration the requirements of such systems. The name of the network is LOCHNESS. It is a distributed system, consisting of several subsystems. Each subsystem is controlled by a minicomputer and is devoted to a special control function, to some kind of data acquisition or to man-machine communication. In the last case the subsystem control computer is functioning as a supervisory control computer. As subsystem control computers we are using 16-bit TPA minicomputers (TPA-1148, TPA-11/440).

A subsystem may or may not contain microprocessor based control stations. In LOCHNESS the control stations are intelligent CAMAC crate controllers based on Intel 8080 microprocessors.

```
                    coaxial cable
H=========================================================H
      !                        !                        !
      !          W             !          W             !
  -----------    I c      -----------     I        -----------
  !         !    I o      !         !     I c      !         !
  !   TPA   !----I a      !   TPA   !----I o       !   TPA   !
  !         !    I x      !         !     I a      !         !
  -----------    I i      -----------     I x      -----------
                 I a                      I i
     -------     I l         -------      I a
     ! ICC !-----I           ! ICC !-----I l
     -------     I c         -------      I
                 I a                      I c
     -------     I b         -------      I a
     ! ICC !-----I l         ! ICC !-----I b
     -------     I e         -------      I l
                 I                        I e
                 M           -------      I
                             ! ICC !-----I
                             -------      I
                                          M
```

Fig. E-3. Sample layout

The communication medium is a coaxial cable both within a subsystem and between the subsystems. A sample lay-out can be seen in *Fig. E-3*. Each subsystem uses a separate coaxial cable segment and the subsystems are connected by a common segment. The maximum length of a cable segment is 1 km, the transfer rate is 1 Mbit/s, and the cable is isolated from the machines up to 15 kV DC.

NETWORK LAYERING

LOCHNESS is designed according to the layered structure of the ISO Open System Interconnection architecture [1], but some layers are not implemented if their functions are not required, while others with strongly reduced functionality are incorporated into the neighbouring ones. As a by-product, this simplification results in an increased efficiency.

O S I	L O C H N E S S
Application	- Terminal Communication - File Transfer Services - Remote Terminal Facility
Presentation	Not implemented
Session Control	
Transport Control	Interface routines LOCHNESS Service Program and program of the ICC interface
Network Control	
Logical Link Control	RSX Driver + microprogram and program of the ICC interface
Media Access Control	Interface hardware and microprogram
Physical Layer	Interface hardware

Fig. E-4

Comparison of OSI and LOCHNESS layering

The correspondence between the OSI reference model and LOCHNESS is shown in *Fig. E-4*. In the figure the three layers of the IEEE 802 project are shown in place of the two lowest OSI layers.

NETWORK UTILITIES

In the TPA minicomputers at the application layer four services are available to the users:

- With the help of the File Transfer Utility program files can be transferred between any two minicomputers connected to the network. The File Transfer Utility supports remote director's listings as well as the submission of command files for execution.

- With the help of the Remote Terminal Support program any terminal can be connected to a remote minicomputer and can be used in the same way as a local one connected to that computer.
- With the help of the Terminal Interchange Utility messages can be exchanged or a dialogue can be pursued between any two minicomputer terminals.
- With the help of the Virtual Device Package a remote physical device (disk, magnetic tape or printer) can be used through the network in a completely transparent way.

These services are generally offered in most network software systems. The most interesting application layer, a very important one, is a distributed Process Control Data Base system. It can manipulate data in the memory, on the disk of a local or remote minicomputer, or in the memory of a remote intelligent CAMAC crate controller. Data can be accessed through the network in a transparent manner.

EXCHANGE OF DATA BETWEEN USER PROCESSES

LOCHNESS is a virtual circuit oriented network. Each logical link is a temporary data path (virtual circuit) connecting two processes. The two programs can exchange data over the logical link, until one of them decides to break the connection. The most important functions of the transport layer are the creation and deletion of the virtual circuits or logical links.

A logical link is dynamically created and deleted between two processes running in the minicomputers if both processes agree to communicate. The two processes must have a preliminary dialogue with the help of the transport layer. In this three part handshaking procedure (the two processes and the transport layer) each program recognizes and agrees to be linked to the other task.

While the flexibility in setting-up of virtual circuits is necessary in the case of the minicomputers, it is not needed for the intelligent CAMAC crate controllers, where a more or less permanent supervisory control function is provided by the subsystem computer. Therefore we have introduced the concept of static (prefixed) logical links. In this case all the allowed pairings of processes are listed in a control table and only the process name and the free or busy state of the requested port are checked by the transport layer in the minicomputer. If the port is not used for any existing connection, it is made available for the requested logical link. If the port is already used by an other task, the connection is rejected.

The allocation of the ports for the prefixed logical links is the task of the system manager(s). It can be done during the generation of the control tables describing the configuration of the communicating systems. Nevertheless, all this is hidden from the user processes, they should request the connection in the same way in both cases.

COMMUNICATION CONTROLLERS AND LINE ARBITRATION IN LOCHNESS

The communication controllers provide for the error-free, fast transfer of data between the memories of the computers connected to the LOCHNESS network. The line arbitration method is also implemented in the communication controllers. The control of the access to the communication line is completely distributed.

The line arbitration mechanism used in LOCHNESS is a modified CSMA/CD algorithm. The CSMA/CD technique is supplemented with a slotting system, which provides for fast acknowledgement and quick retransmission of the frames in case of transmission errors. The slotting scheme can be used to implement contention free multiframe control sequences, too.

As data can be sent over existing logical links only, this provides for a selective flow control facility, which works on each connection independently from the others, i.e. the buffer requirements of the individual connections do not interfere with each other. This selective flow control ensures that no data will be transmitted through a connection until a receiving buffer is available, and the data are placed immediately to the buffer of the receiving task, no internal copying of the data is required. This selective flow control is strongly supported by the hardware providing the facility of the contention-free multiframe sequences.

The arbitration method as well as the logical link control is described in more details in Ref. [2].

NETWORK EFFICIENCY

A main design goal was to provide for the effective utilisation of the transmission bandwidth of the common bus. The following measurement data show, to what extent this goal was reached.

The nominal transmission speed of the bus is 1 Mbps. If the arbitration and protocol (framing and handshaking) overhead is subtracted, 800 kbps useful data could be sent over the bus. Of course, no pair of processes can acquire such big share of the transmission capability.

According to our measurements: with clever programming - if no other communicating parties are present - two communicating processes can transfer up to 640 kbps useful data over the communication line from memory to memory.

At the message length of 512 bytes already two minicomputers can utilize the cable capacity upto 65%, and two independent pairs upto 79%. This is much higher than the data rate which could be reached if the data to be transmitted were to be read from disk, or they were to be written to disk. Thus if any reasonable data source or sink speed is assumed, a considerable number of simultaneous logical links can communicate at "full" speed over the communication bus.

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PCDB - DISTRIBUTED DATA BASE MANAGEMENT SYSTEM FOR PROCESS CONTROL

G. Juhász, K. Kovács, I. Sári

For many years our institute has accumulated experience in developing industrial and laboratory process control systems. This experience shows that, on the one hand, the amount of data to be acquired by such systems is becoming greater and greater and, on the other hand, the software systems to be produced are also becoming increasingly more complex. This large amount of data brings about high management costs, which can be kept within reasonable limits only when the number of data structures used is kept small. Today's solution to this problem is the concept of the process control data base.

DISTRIBUTED DATA

PCDB ("Process Control Data Base Management System") allows the user to perform various operations in a distributed process control data base, where the data are distributed amongst subsets (called local bases) stored at various sites (mini and micro computers), geographically dispersed but interconnected by a high-speed communication network [1].

The minis are hierarchically on the same level. However, every microcomputer is supervised by a mini. The PCDB services are available for the minicomputer users only. PCDB considers the micros as intelligent peripheral devices of a given mini, although the mini-mini and mini-micro network connections are similar [2]. In the present realization minicomputers are TPA-11 or compatible processors, microcomputers are INTEL 8080-based Intelligent ("CAMAC") Crate Controllers ("ICCs") interconnected by the "LOCHNESS" [3].

```
. . . ----------------------------------- . . .    [
         I                         I               [ NETWORK
         I                         I               [
         I                         I
    ------------            -------------
    I          I            I           I          [
    I          I            I           I          [
    I   PCDB   I            I   PCDB    I          [ TPA-S
    I          I            I           I          [
    I          I            I           I          [
    ------------            -------------
         I                         I               [
  ...--------------...    ...---------------...    [ NETWORK
      I        I              I          I         [
  --------  --------      --------  --------
  I      I  I      I      I      I  I      I       [ INTELLIGENT
  I PCDB I  I PCDB I      I PCDB I  I PCDB I       [ MEASURING
  I      I  I      I      I      I  I      I       [ SUBSYSTEMS
  --------  --------      --------  --------
   I I I     I I I         I I I     I I I         [ MEASURING
   o o o     o o o         o o o     o o o         [ POINTS
```

A typical process control system architecture

The application programs themselves are distributed amongst the various sites of the network. The distributed data base is the common resource of user programs.

RELATIONAL MODEL

Our data base management system is based on the relational model where the data have to be organized in simple tables [4,5]. PCDB ensures data consistency, decoupling of data from the application programs (program independent data), and the independence of programs from physical and logical data structures.

The data base consists of a set of declarations which describe the logical and physical data structures, called the schema, and of tables which contain the data, called relations. The rows of these tables are called "records" while the columns are denoted as "attributes" [4].

The schema describes the relation and its attributes (e.g. type, byte position and size for each attribute, etc.). PCDB includes different types of attributes: integer (1, 2 and 4 bytes), real (4 and 8 bytes), string and bit string. Numeric attributes can be arranged in vectors.

DATA MANIPULATIONS

```
                      ++++++++++++
                      +          +
                      +   USER   +
                      +   TASK   +
                      +          +
       ---------------+          +-------------------
       I..............+   RMR    +..................I
       I..............+ ROUTINES +..................I
       I..............++++++++++++..          ......I
       I..........................   P C D B   .....I
       I..........................            ......I
       I................................................I
++++++++++++++++++........------------------.........I
+      I      R  +........I                 I.........I
+      I      O  +........I  DATA IN CORE   I.........I
+ USER I  R   U  +........I                 I.........I
+      I  M   T  +........I-----------------I.........I
+ TASK I  R   I  +........I                 I.........I
+      I      N  +........I  DATA ON DISK   I.........I
+      I      E  +........I                 I.........I
+      I      S  +........I-----------------I.........I
++++++++++++++++++........I                 I.........I
       I..................I    NETWORKS     I.........I
       I..................I                 I.........I
       I..................I         I       I.........I
       I..................I  DATA   I  DATA I.........I
       I..................I         I       I.........I
       I..................I   IN    I   IN  I.........I
       I..................I   ICC   I  TPA  I.........I
       I..................I         I       I.........I
       I..................------------------..........I
       I................................................I
       --------------------------------------------------
```

PCDB architecture

Application programs can access data records or columns by means of the Relation Manipulation Routines "RMR", independently from the actual location of the relation.

Records or columns can be referenced by a sequence number or by a key (e.g. process variable identifier). RMR routines may be called from high level language (FORTRAN, BASIC, PASCAL) and from assembly language (MACRO-11) programs.

```
                                              ATTRIBUTES
                                             /    I     \
                                            /     I      \
                                           /      I       \
                                    ---------------        ------
                      RECORD NO.1 I      I       I . . . I     I
                                    ---------------        ------
                      RECORD NO.2 I      I       I . . . I     I
                                    ---------------        ------
                             .      .       .              .
                             .      .       .              .
                             .      .       .              .
                                    ---------------        ------
++++++++++==========                I      I       I       I     I
+        -   RMR    =               ---------------        ------
+        -  GETREC  =               I      I       I       I     I
+  USER  -  GETNXT  =               ---------------        ------
+        -  UPDCUR  =            ---------------        ------
+        -  UPDNUM  = ---  I XXXX I YYYYY I  . . . I ZZZ I
+  TASK  -  PUTNUM  =            ---------------        ------
+        -  DELCUR  =               ---------------        ------
+        -  DELREC  =               I      I       I       I     I
+        -  APPEND  =               ---------------        ------
++++++++++==========                I      I       I       I     I
                                    ---------------        ------
                                    I      I       I . . . I     I
                                    ---------------        ------
```

PCDB record access

```
                          ATTRIBUTES
                   /         I         \        \
                  /          I          \        \
                 /           I           \        \
             ---------------           ---------------
RECORD NO.1  I      I      I . . . I      I          I
             ---------------           ---------------
RECORD NO.2  I      I      I . . . I      I          I
             ---------------           ---------------
      .          .       .               .
      .          .       .               .
      .          .       .               .
             ---------------           ---------------
             I      I      I           I      I          I
             ---------------           ---------------
             I      I    ---------     I      I    ----------
             ----------I XXXXX I       ----------I YYYYYYY I
             I      I    ---------     I      I    ----------
             ----------I XXXXX I       ----------I YYYYYYY I
             I      I    ---------     I      I    ----------
             ----------I XXXXX I       ----------I YYYYYYY I
             I      I    ---------     I      I    ----------
             ----------I XXXXX I       ----------I YYYYYYY I
             I      I    ---------     I      I    ----------
             ----------I XXXXX I       ----------I YYYYYYY I
                 .       ---------               .  ----------
                 .                               .
             ---------------           ---------------
             I      I      I . . . I      I          I
             ---------------           ---------------
             I      I      I . . . I      I          I
             ---------------           ---------------
                                   I
                                   I
                      ++++++++============
                      +        -   RMR    =
                      + USER   -  GETITV  =
                      +        -  GETLST  =
                      + TASK   -  UPDITV  =
                      +        -  UPDLST  =
                      ++++++++============
```

PCDB column access

PCDB FEATURES

In process control applications the response time may be critical so PCDB supports core resident data handling [5].

PCDB has an efficient resource handling mechanism to ensure data consistency and support continuous operation without deadlock.

In the case of transient disk, memory or network system errors PCDB executes a special recovery procedure to maintain a non-interrupted service.

A number of PCDB utilities help the user to create, save, restore, examine and modify data either in interactive way or from programs.

PCDB is designed to support minicomputers of TPA-11 family under the DOS-RV/DOS-RV-PLUS operating systems. PCDB requires 4.5K to 40K words of main memory.

PCDB is a component of a set of process control oriented software tools developed for minicomputers. For example, a sophisticated operator communication facility can use PCDB services (DICOM).

PCDB allows LOCHNESS to be replaced by DECnet for TPA interconnections.

APPLICATIONS

PCDB has been in use in the following industrial systems:

- the National Telemechanical System for gas pipeline control,
- the Control System for Budapest Waterworks and
- the North Hungarian Power Distribution Control System.

PCDB can be used in the laboratory environment as well:

- the automatic control system of the T-15 tokamak nuclear fusion facility is to use PCDB.

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NATIONAL TELEMECHANICAL SYSTEM

J. Cser, L. Szőnyi

The National Telemechanical System (NTS) is an intelligent hierarchical network for data acquisition and remote control of gas pipelines in Hungary. It contains the National Gas Dispatcher Centre (NGDC), and four Regional Gas Dispatcher Centres (RGDC).

The control system has the following hierarchical levels:

- NGDC;
- communications between NGDC and the four RGDCs;
- RGDCs;
- Regional Telemechanical Centres (RTMC), host controllers;
- telemechanical communications line;
- telemechanical stations;
- technological instrumentation.

Our institute has designed and delivered the computers for NGDC and RGDCs. The block diagram of NTS is illustrated in *Fig. E-5*.

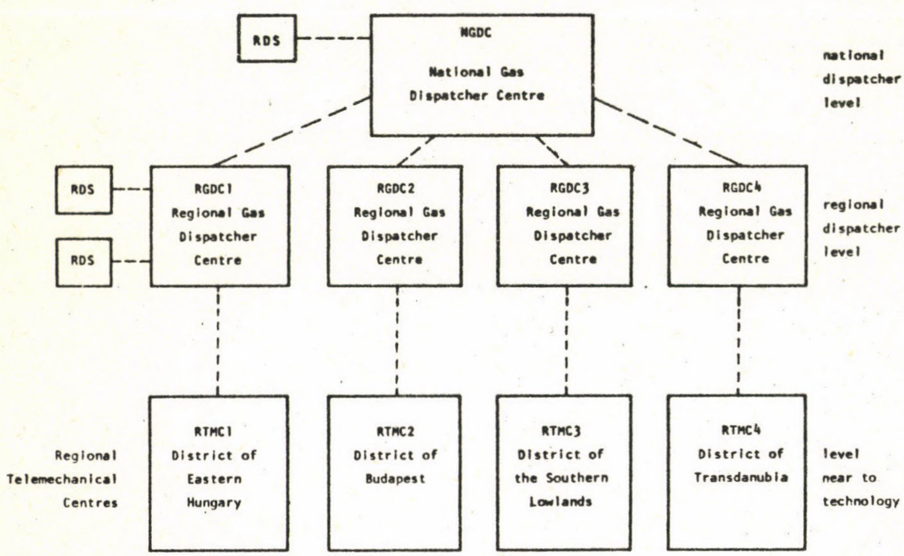

Fig. E-5

Block diagram of NTS

Main tasks of the NGDC are:

- information supply for operative control at the national level;
- control of the technological parameters of primary importance;
- supervision of the RGDCs;
- supply of data for control authorities at higher levels;
- post-evaluation of technological tasks.

Main tasks of the RGDC are:

- supply of basic and originated data for effective and reliable operative control;
- technological control;
- controlled interrupts;
- administration and statistics at lower levels;
- post-evaluation of technological tasks.

Computer systems in the dispatcher centres execute eventual and systematic data collection, handle disturbances and errors, process data for different views, and archive and save data. All of these operations refer to a data base containing current and past status information from the technology. They generate, read-out and manipulate the data base.

The computer systems are based on TPA-1148s equipped with background stores for program and data storage, archivation and saving of data, and with alphanumeric and semigraphic displays for man-machine interaction, printers and communication devices for coupling the technology, the RGDCs and the NGDC together.

For the sake of higher reliability, computers and host controllers are duplicated, and the task execution can be directed from one machine to the other. Some peripherals can be assigned to any of the two machines according to task distribution. A microprocessor-based intelligent supervisor unit monitors the operating status of the computers, and changes the peripheral assignment, if necessary. The block diagram of the computer system at NGDC is illustrated in *Fig. E-6*. Computer systems at RGDCs differ from it in the presence of the technological connections, and in the number of communication lines and Remote Dispatcher Stations (RDS).

The first RGDC was installed in the middle of 1983, and the whole network, including the NGDC and all the four RGDCs, was put into operation in June 1984. Since that time NTS has operated reliably and has been contributing to a more sophisticated and a more economical gas supply of Hungary.

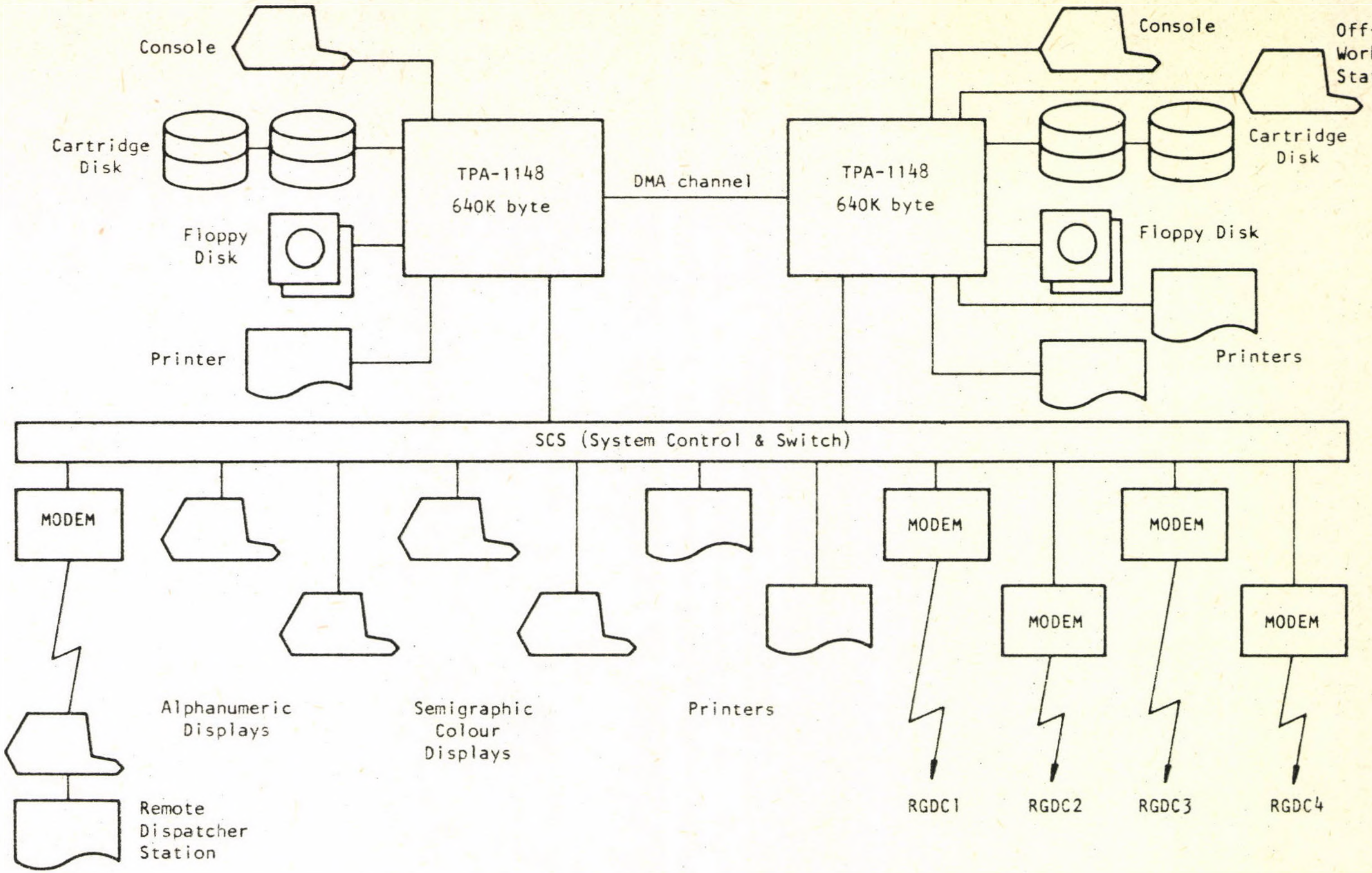

Fig. E-6

Block diagram of NGDC

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COMPUTING CENTRE (SzK)

The Computing Centre has been functioning as an independent department since 1980. Its main tasks are running the central computing facilities and carrying out scientific research in related subjects.

The mainframe computer is an ES-1040 installed in 1977, with 1 MB main memory and 640 MB disk storage. There are 20 videoterminals attached to a TPA 70 front-end processor and driven by the Conversational Editor and Remote User's Support (CEDRUS) system which was developed in KFKI.

Some relevant data pertaining to the computing services are as follows:

Year	*Effectivity*	*Machine time available for user's jobs (hours/year)*	*Number of jobs/year*
1983	*94.36*	*7661*	*80551*
1984	*95.07*	*7865*	*76092*

One of the paper tape units has been recently replaced by an intelligent casette data recorder of type NEO-202, wich is currently in use in the laboratories of the institute. Now data are processed from a magnetic casette deck instead of a paper tape input in order to enhance reliability of data transfer.

Since the present requirements for memory and speed exceed the inherent limitations of the present system, the purchase of a new, more powerful computer is now in progress.

In preparation for the new ES-1045 computer, a good deal of activity is directed towards the installation: system generation, program implementation and planning and development of a new terminal network.

The development of the hardware and software components of a local area network connecting the minicomputers in the different laboratories with the host computer is now going on. The network will be capable of sending files and jobs to and from the minicomputers and the host computer. This work is being done in cooperation with KFKI's Institute of Measurement and Computing Technique.

Part of the research done in the Computing Centre aims at running the computer as effectively as possible. A program (MONFORT) for monitoring the central processor usage of FORTRAN programs has been developed. The results are useful in searching for those critical parts of a program that use the most CPU time and need further optimization.

The Waterloo FORTRAN compiler WATFIV is now installed, thus giving invaluable help to FORTRAN programmers in debugging their programs.

Research in the field of symbolic computing is being continued. Some new programming systems have been made available for users. Among them the CAMAL system,the REDUCE3 system, which is employed for calculations in theoretical physics, are of special interest.

The development of user programs is supported by a number of program libraries that contain thousands of programs and subroutines for a wide range of applications. International cooperation has made it possible to obtain many useful application programs, thus extending our program library. Among them are the IMSL, SL-MATH, CERN, Computer Physics Communications Program Library, EISPACK, RUTHERFORD and HARWELL Libraries. The basic tool of text formatting is the program DRUNOFF. The Computing Centre has been providing SDI services for our institute's library for about twelve years.

The plotter subroutine package (containing over 50 routines) has been revised and a new manual was issued in Hungarian. As a part of the work, a line-plotting procedure was developed which is capable of handling discontinuities, singular points and abrupt changes of curves.

Also, the user community is helped by a newly written ES-1040 computer manual and a monthly periodical, carrying the news of the Computer Centre.

The computerized processing of the European Physical Society membership registry is done here by using the IDMS database management system. We also participate in the development of another large-volume database application: a stock management and production control support system based on the database management system DBMS-11.

In another research and development program we have joined with four other leading Hungarian institutions to develop an Ada compiler system for mini and mainframe computers. Our department has contributed to this project by planning and realizing the Ada Library (together with colleagues from SZÁMALK).

The structure of kernel languages has been studied, with respect to the Chomsky-hierarchy and their properties in the abstract family of formal languages.

We developed a new efficient graph colouring algorithm for scheduling problems. Based on this algorithm, a computer program for school timetable construction has been successfully tested in real life situations.

A computer program for calculating the molecular force field using the generalized inverse of matrices has been incorporated into the Computer Physics Communications Program Library.

In numerical matrix algebra, the structure of tridiagonal matrix inverses has been studied and results concerning the zero division problem in matrix conjugate direction algorithms have been obtained.

In collaboration with the Joint Institute for Nuclear Research, Dubna, USSR, we have worked out some algorithms and programs for the solution of some problems in physics. The actual topics were mathematical modelling of data processing, numerical methods of discretization and rational approximation of functions. For example, for discontinuous functions it has been shown that the generalized Padé approximation for the function sgn(x) has a smaller Gibb's constant than that of a classic Fourier series.

APPLICATION OF THE METHOD OF GENERALIZED INVERSE OF MATRICES FOR COMPUTATION OF MOLECULAR FORCE FIELDS

Barbara Gellai

1. INTRODUCTION

The concept of the generalized inverse [1-2] of matrices and the theory of its application to least squares problem are well known [3-5]. However, the practical usefulness of the theory for physical problems is not so well established.

It is well known [3] that the estimation $\hat{\underline{x}}$ of the solution of a system of equations obtained by the generalized inverse is not unbiased. Namely, if the m x n matrix $\underline{\underline{A}}$ of the system is of rank r, (r < n), then

$$\varepsilon\hat{\underline{x}} = \varepsilon(\underline{\underline{A}}^{+}\underline{b}) = \underline{\underline{A}}^{+}\varepsilon b = \underline{\underline{A}}^{+}\underline{\underline{A}}\underline{x} \ . \tag{1}$$

where ε is the expected value operator and $\underline{\underline{A}}^{+}$ is the generalized inverse of $\underline{\underline{A}}$.

The estimation of the elements of the vector $\underline{x}$ which belong to the unit block of the matrix $\underline{\underline{A}}^{+}\underline{\underline{A}}$ is unbiased, while the same is true only for linear combinations of the other elements of $\underline{x}$.

The aim of the present paper is to demonstrate the usefulness of the method of generalized inverses in the computation of molecular force fields, and to demonstrate how the structure of the matrix $\underline{\underline{A}}^{+}\underline{\underline{A}}$ can serve as a guide to determining the definiteness of the resulting force field parameters.

In the next section a brief review of the relevant published results is given. In the following section numerical results for the molecule dymethylmercury are presented.

2. MATHEMATICAL BACKGROUND

Let $\underline{\underline{A}}$ be a real m x n matrix of rank r, (r < n). There exist matrices $\underline{\underline{U}}_r$, $\underline{\underline{\Sigma}}_r$ and $\underline{\underline{V}}_r$ such that [6]

$$\underline{\underline{A}} = \underline{\underline{U}}_r\underline{\underline{\Sigma}}_r\tilde{\underline{\underline{V}}}_r \tag{2}$$

where $\underline{\underline{\Sigma}}_r$ is an r x r positive diagonal matrix with the elements σ_i with the property

$$\sigma_1 \geq \sigma_2 \geq \dots \sigma_r \geq \sigma_{r+1} = \sigma_n \dots = 0 \ . \tag{3}$$

The σ_i' s are the non-negative square roots of the eigenvalues of the matrix $\tilde{\underline{\underline{A}}}\underline{\underline{A}}$ and are called the singular values of $\underline{\underline{A}}$. The matrix $\underline{\underline{U}}_r$ is an m x r and $\underline{\underline{V}}_r$ is an n x r matrix, which satisfy the relation

$$\tilde{\underline{\underline{U}}}_r\underline{\underline{U}}_r = \tilde{\underline{\underline{V}}}_r\underline{\underline{V}}_r = \underline{\underline{I}}_r, \tag{4}$$

and which consist of the eigenvectors belonging to the r non-zero eigenvalues of the matrices $\underline{\underline{A}}\tilde{\underline{\underline{A}}}$ and $\tilde{\underline{\underline{A}}}\underline{\underline{A}}$, respectively. The matrices $\underline{\underline{U}}_r$ and $\underline{\underline{V}}_r$ can be obtained without solving the related eigenvalue problems [7].

The ratio

$$\mathrm{cond}(\underline{\underline{A}}) = \sigma_1/\sigma_r \tag{5}$$

is the condition number of the matrix $\underline{\underline{A}}$. The smaller the condition number of a matrix the better is its condition with respect to matrix inversion.

Using the decomposition defined by eq. (2) the unique minimal (minimum norm) least squares solution of an incompatible m x n system of equations with the matrix $\underline{\underline{A}}$ can be written as [5]

$$\underline{x} = \underline{\underline{V}}_r\underline{\underline{\Sigma}}_r^+\tilde{\underline{\underline{U}}}_r\underline{b} = \underline{\underline{A}}^+\underline{b} \ . \tag{6}$$

Here,

$$\underline{\underline{A}}^+ = \underline{\underline{V}}_r\underline{\underline{\Sigma}}_r^+\tilde{\underline{\underline{U}}}_r \tag{7}$$

is the generalized inverse of the matrix $\underline{\underline{A}}$, while the elements of $\underline{\underline{\Sigma}}_r^+$ are σ_i^{-1}, (i = 1,2, ... r).

3. NUMERICAL RESULTS AND DISCUSSION

The relationship between the observed spectroscopic data $\nu_i (i=1,2,\dots,m)$, and the force constants f_j, ($j = 1,2, \dots, n$; $m > n$), is nonlinear. The weighted squares of residual $\tilde{\underline{r}}\underline{\underline{W}}\underline{r}$ should be minimized such that

$$\tilde{\underline{r}}\underline{\underline{W}}\underline{r} = \Delta\tilde{\underline{\lambda}}\underline{\underline{W}}\Delta\underline{\lambda}, \tag{8}$$

where

$$\underline{r} = \Delta\underline{\lambda} - \underline{\underline{J}}\Delta\underline{f} \ . \tag{9}$$

Here, J is the Jacobian matrix, which is often close to being singular because the isotope product role [8] causes some frequencies to be related. Here λ_i is the frequency parameter: $\lambda_i = 4\pi^2c^2\nu_i^2N^{-1}$, where c is the velocity of light and N is the Avogadro number.

We have successfully applied [9-11] the theory described in section 2 to this problem and have also developed a complete FORTRAN program [12] to performe the computations.

The force field calculation of the symmetry species "a" of the molecule $(CH_3)_2Hg$ has been used as a test case. Because of the molecular symmetry, eight force constants out of the twelve should be refined independently. The statistical weights $w_i (i = 1,2,...,m)$, were chosen to be $1/\lambda_i$. The Jacobian matrix is almost exactly singular (see *Table 1*); there is a well defined gap between the n-th and the (n - 1)-th singular

Table 1

Singular values of the Jacobian matrix of the molecule dimethylmercury

Method applied	*Singular values*				
Generalized inverse	*3.42706*	*0.82217*	*0.58725*	*0.34346*	*0.22457*
	0.16596	*0.74191×10^{-1}*	*0.39929×10^{-11}*		
Least squares with constraint $F_{13} = 0$	*3.42674*	*0.82189*	*0.58271*	*0.34336*	*0.22452*
	0.16553	*0.70288×10^{-11}*			
Least squares with constraint $F_{12} = 0$	*3.41193*	*0.81352*	*0.56250*	*0.33978*	*0.22465*
	0.16326	*0.29020×10^{-1}*			
Least squares with constraint $F_{56} = 0$	*3.42706*	*0.58725*	*0.34346*	*0.20965*	*0.16596*
	0.74191×10^{-1}	*0.58598×10^{-11}*			

value. Due to the uncertainty of the measured spectroscopic data the elements of the Jacobian proved to be accurate to the second decimal place. Replacing the last singular value by zero, the rank proved to be constant during the iteration (see *Table 2*). It should be noted that a well defined gap between two singular values does not necessarily exist and the singular values of the Jacobian matrix may gradual approach zero. In this case a determination of numerical rank is rather difficult and the theory needs further investigation.

The symmetrical projector matrix (see *Table 3*) shows that all force constants can be regarded as determined except for F_{12} and F_{13}. Their values can be chosen freely or assigned on the basis of some physically relevant force field model. Applying the constraint $F_{12}=0$ and $F_{13}=0$ the Jacobian in both cases became well conditioned and the method of the generalized inverse thereby went over into the usual least squares method (see *Table 1*). The force field results with the constraint $F_{13} = 0$ are compared with the results obtained by the method of generalized inverse in *Table 4*.

Table 2

Changes of some characteristic quantities during the iteration when applying the method of generalized inverse

Cycle	*Condition number*	$\|\|\Delta f\|\|_2$	$\underline{r}\underline{\underline{W}}\underline{r}$	$\Delta\underline{\lambda}\underline{\underline{W}}\Delta\underline{\lambda}$
1	46.209	0.52541	0.16928×10^{-2}	0.55633×10^{-1}
2	41.931	0.29188	0.76969×10^{-2}	0.18896×10^{-1}
3	40.957	0.24395	0.20960×10^{-3}	0.48509×10^{-3}
4	40.951	0.58983×10^{-1}	0.17174×10^{-3}	0.171148×10^{-3}
5	40.951	0.13269×10^{-3}	0.17147×10^{-3}	0.17147×10^{-3}
The last three singular values				
	0.16596	0.74191×10^{-1}	0.39929×10^{-11}	
	0.19710	0.78908×10^{-1}	0.58451×10^{-10}	
	0.19395	0.81057×10^{-1}	0.40753×10^{-10}	
	0.19434	0.81064×10^{-1}	0.37629×10^{-10}	
	0.19434	0.81064×10^{-1}	0.39510×10^{-10}	

The result obtained with the constraint $F_{12} = 0$ was close to the one obtained with $F_{13} = 0$. On the other hand, if the relatively small F_{56} (see *Table 4*), the value of which proved to be strongly determined (see *Table 3*), was constrained to be zero the Jacobian matrix remained singular (see *Table 1*). The fit to the spectroscopic data was found here to be worse by one order of magnitude either than that obtained by the method of generalized inverse or that obtained by applying the previous constraints.

The method proved to be successful when applied to the symmetry species E and it indicated the indeterminacy of the force constants that can not be determined from vibrational frequencies alone. Here, other data such as Coriolis interaction constants are needed if more meaningful values are to be obtained.

The above results prove that the structure of the projector matrix $\underline{\underline{A}}^{+}\underline{\underline{A}}$ is a useful guide for establishing the degree of indeterminancy of the individual force field parameters.

Table 3

Elements of the symmetrical projector matrix $J_r^{+}J_r$ *(r = 7)*

0.988	-0.040	0.103	0.006	-0.001	-0.010	0.000	0.000	F_{11}
	0.873	0.329	0.020	-0.004	-0.032	0.000	0.000	F_{12}
		0.151	-0.051	0.011	0.083	0.000	0.000	F_{13}
			0.997	0.001	0.005	0.000	0.000	F_{22}
				1.000	-0.001	0.000	0.000	F_{23}
					0.992	0.000	0.000	F_{33}
		Symm.				1.000	0.000	F_{56}
							1.000	F_{66}

Table 4

Initial and final set of force constants in terms of symmetry coordinates (mdynÅ^{-1})

Symm. species	Force constants	Initial set	Results with method of gen. inverse	Results with constraint F_{13} = 0
	F_{11}	4.930	4.758±0.045	4.741±0.052
	$\hat{F}_{12}$	0.050	-0.310±0.050*	-0.361±0.059
a_{1g}	F_{13}	0.010	-0.133±0.025*	0.0
	F_{22}	0.353	0.382±0.010	0.390±0.012
	F_{23}	-0.120	-0.169±0.028	-0.172±0.027
	F_{33}	2.480	2.409±0.029	2.403±0.029
	F_{44}	4.930	4.758±0.045	4.741±0.052
	$\hat{F}_{45}$	0.050	-0.310±0.050*	-0.361±0.059
a_{2u}	F_{46}	0.010	-0.133±0.025*	0.0
	F_{55}	0.353	0.382±0.010	0.390±0.012
	F_{56}	-0.120	-0.075±0.008	-0.078±0.008
	F_{66}	2.580	2.370±0.026	2.364±0.027

*Linear combinations of F_{12} and F_{13}

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DEVELOPMENT ENGINEERING (MSZI)

One of the main activities of the Development Engineering Division (MSzI) is the development and manufacture of unique mechanical equipment and electronic systems to satisfy both the internal needs of KFKI and the needs of the various fields of the national economy.

In addition, there are basic and applied technical research activities, pursued jointly with other institutes of KFKI. MSzI also manages the utility systems (heat, electric energy, water, gas, etc.) of KFKI as well as a number of other activities ranging from building investments to technical maintenance.

The active participation in the development of the mechanical and electronical subsystems of the project VEGA was the most important activity of MSzI during the period 1983-84. Our high quality workmanship met the special technical and environmental requirements, and the Hungarian instruments were, as planned, on board of the two VEGA space probes that were successfully launched in December 1984. Further R&D activities of the Development Engineering Division are outlined below.

The first practical results in mechanical engineering using Computer Aided Design techniques were achieved in 1983. The software development has been based on writing our own original programs as well as on software exchange with other research institutes [e.g., the Scientific Instrumentation Division of the Nuclear Research Institute near Dresden (GDR), the Technical University Budapest and the Computer and Automation Research Institute of the Hungarian Academy of Sciences].

Programs have been developed to maintain high standards and effeciency in our own engineering design activities. Most of our results were obtained in the fields listed below:

- Geometric modelling of parts, program system DIM7;
- Finite element analysis package, program system MESH;
- Geometric design and stressing of machine parts;
- Dynamic simulation of technical systems using the program system DIVASYM.

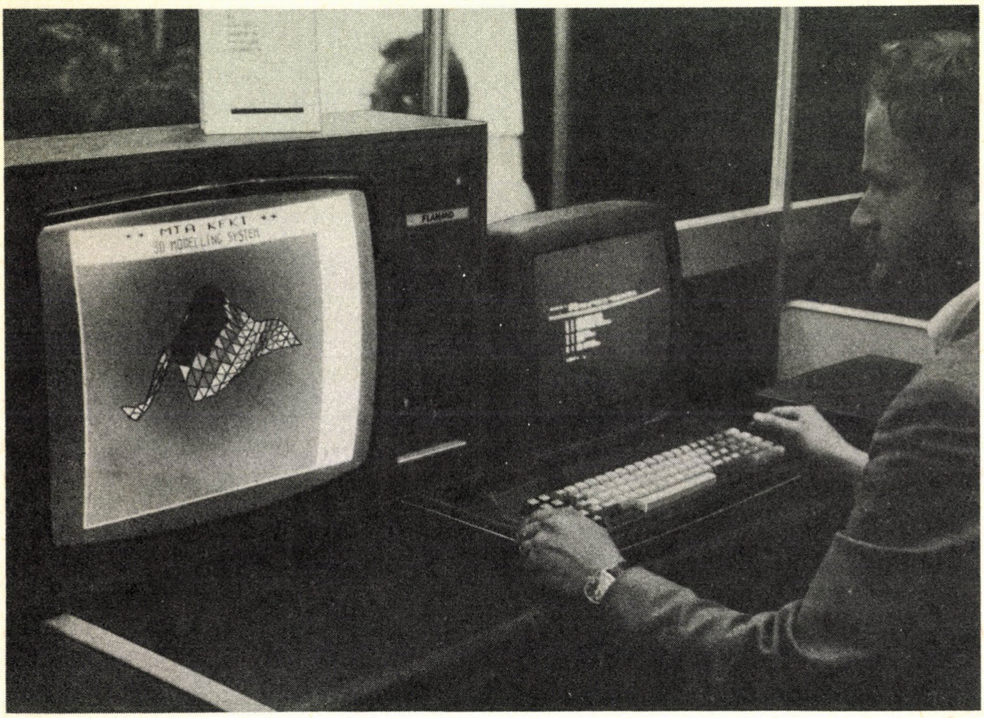

Fig. G-1

Computer Aided Design Workstation

The development of a high pressure oxidation system is a representative example among the devices built for the silicon based technology using a complex mechanical and electronical design approach. The system is built to perform dry and wet oxidation and heat treatment of silicon wafers in an inert gas atmosphere.

The equipment consists of a stainless steel high pressure vessel with double walls, a three zone furnace for the oxidation process, and a gas system.

The automatic operation and the safety interlocking system is controlled by a microprocessor based control unit. Manual operation is also possible.

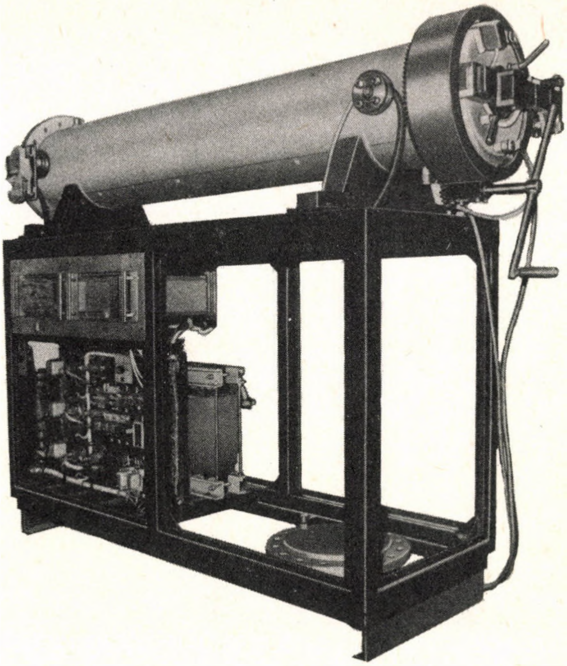

Fig. G-2

High pressure oxidation equipment under construction

The main technical data of the high pressure oxidation system are

Highest pressure in the working zone	10^6 Pa (10 bar)
Operating temperature	600-1200 °C
Length of the homogeneous zone	500 mm
Maximal temperature deviation within the homogeneous zone	± 0.5 °C

This microelectronical technological system is capable of handling larger batches of wafers as well.

An other example of microelectronical technological equipment is our mask and wafer cleaning system for the automatic washing of microelectronic photomasks and wafers. The fixing and rotating of the wafers, the injection of the cleaning, drying and coating agents and the brushing process are all controlled by a microprocessor based electronic unit.

The main technical data are listed below

Maximal wafer size	*5"*
Pressure of deionized chamber	*min.* $1.5x10^7$ *Pa (150 bar)*
Deionized water consumption	*100-200* cm^3*/min*
Wafer heating	*radiant heat*

Three of the most successful projects of the past few years are outlined in the next paragraphs.

DEVELOPMENT OF THE MEASURING AND INTERPRETATION TECHNIQUE OF BODY SURFACE MAPPING

Zsuzsanna Cserjés, A. Csiszár, Gy. Kozmann, F. Pásztor, T. Rochlitz and T. Wolf

The electrical activity of the heart results in a rapidly changing quasi-periodic potential distribution on the body surface. The accurate recording of this field followed by a careful interpretation of the experimental data promises a sophisticated, very powerful non-invasive diagnostic tool for electrocardiology.

In the framework of a long-run research project the KFKI has completed the development of a 64 channel real-time body surface mapping system (CARDIPLOT 64). Up till 1983-84 no such equipment was available on the market. The development was sponsored by the Ministry of Health and the National Council for Technical Development.

The main parts of the system are: a 64 channel optically isolated amplifier set, a fast multiplexer and A/D converter unit, a 32 kword buffer memory for fast intermediate data storage, a TPA/L minicomputer equipped by two cartridge disks, a matrix printer and a graphic display.

CARDIPLOT 64 belongs to the most up-to-date systems, allowing the investigation of single beat as well as averaged beat potential maps of patients at rest. It is also suitable for determining precordial exercise maps. Moreover, the equipment computes from the map data what the signals of the commonly used lead systems would be, thereby allowing a comparison of the information with what would have been obtained with the conventional ECG/VCG methods and body surface mapping *(Fig. G-3)*.

The evaluation of body surface maps requires effective feature extraction methods which provide statistical parameters sufficiently discriminative and, at the same time, physiologically clearly inter-

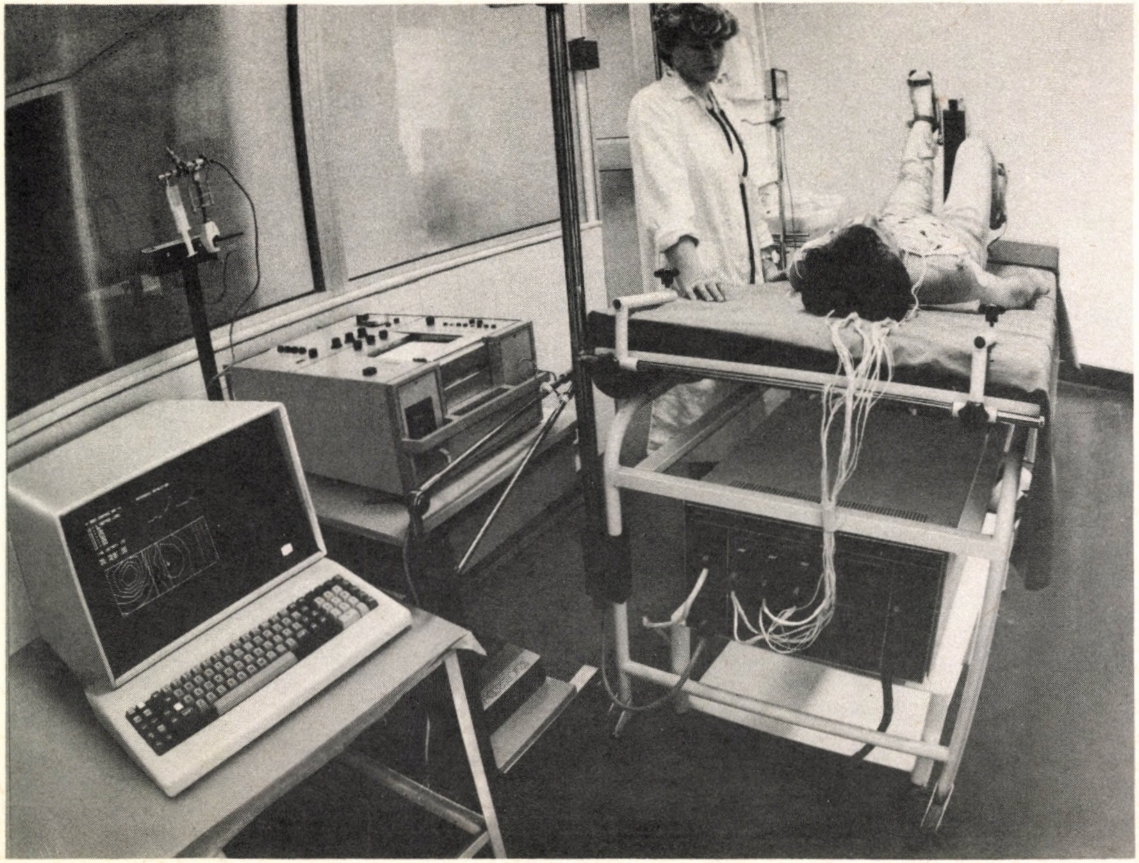

Fig. G-3

CARDIPLOT 64 body surface mapping system in use at the National Institute for Cardiology pretable for a physician. To moderate the difficulties of candidate parameter introduction, a new preprocessing method, which uses isointegral maps of patients corresponding to any two pathological groups to be compared, was developed by our working group.

The method is based on a systematic lead by lead application of the Gnedenko-Koroljuk (G-K) non parametric test of homogeneity.

The result of the procedure is visualized in form of a G-K map where the contour lines encircle those areas on the chest surface where the signals are statistically significantly different in the two groups or, in certain cases, where the signal distributions are even non-overlapping. A surface integral on these subregions considerably reduces the effect of the errors arising from inaccurate electrode positioning and provides favourable (dichotomic) discriminative parameters.

This procedure was successfully applied in a pilot study to discriminate the subgroups of Wolf-Parkinson-White syndrome *(Fig. G-4)* patients.

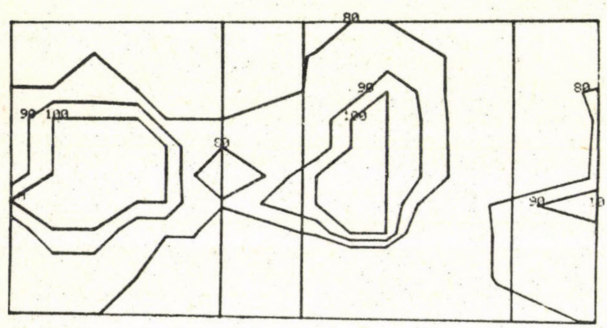

Fig. G-4

Gnedenko-Koroljuk distance map of Wolf-Parkinson-White syndrome patients with left and right side Kent-Palladino bundle. The areas encircled by the contour line 100 show the location of nonoverlapping regions of isointegral maps on a simplified rolled-off chest surface.

We have continued the development of a small-computer model suitable for conceptual studies of electrocardiology. For the time being the thorax is considered as a homogeneous volume conductor with a geometrically regular simplified shape.

For the body surface potential distribution computations the electrical sources of the heart are modelled by lumped equivalent multipolar or multidipolar generators. The instanteneous value of the equivalent source parameters can be estimated by the use of a realistically positioned isotropic heart model, in which the activation propagation is computed analytically on the basis of Huygen's principle. The whole task is transformed into the numerical solution of a linear algebraic system of equations typically with 400-800 unknowns.

The model has been used to study the body surface signs of characteristic excitation events such as the onset of activation waves, collision of the originally separated waves, breakthrough phenomena and the loss in continuity of activation waves in consequence of myocardial infarction. It was concluded that, in contrast with the first two events, the last two result in abrupt slope changes of the ECG curves detectable by linear predictive algorithms.

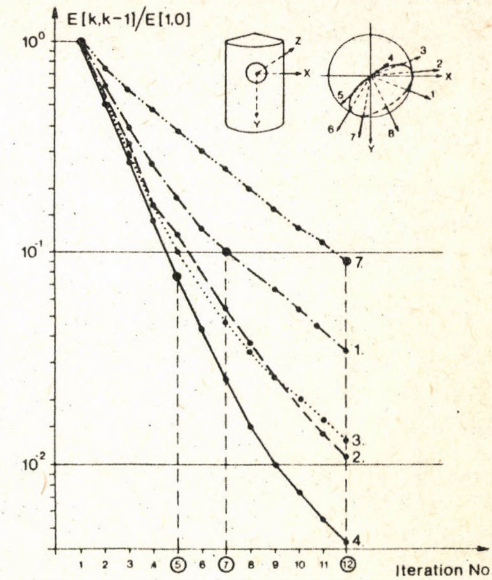

Fig. G-5

Convergence rate of the electrocardiographic forward problem solution by Jacobi iteration in case of 5 dipolar sources. The outline of the chest and heart model is indicated in the right upper corner of this figure, the numbers at the curves correspond to the serial numbers of the dipoles.

Another study revealed that, in the iterative solution of the linear algebraic system of the electrocardiographic forward problem, the number of the necessary iteration steps needed to achieve a prescribed accuracy strongly depends on the location and orientation of the lumped sources (*Fig. G-5*).

MODULAR ELECTRONIC CONTROL SYSTEM FOR TECHNOLOGICAL EQUIPMENT IN MICROELECTRONICS

M. Danka, I. Kovács, A. Rényi and J. Tombor

To ensure the technical quality of the research activities in microelectronics and to solve technological and computer aided measurement problems the control electronics must supply the following: control of temperature; control of magnetic switches, pneumatic valves and gas systems; control of the rotational speed of various motors; automatic safety interlocking systems; programmed transfer and movement of technological wafers.

An electronic modular control system was developed in the Instrumentation Department of MSzI to satisfy these requirements mainly in the field of automatic control of technological equipment in microelectronics.

To complete the set of the usual microprocessor cards additional special modules were developed. The currently available modules are as follows:

- 8080 or 80 based central processing unit with memory and I/O ports;
- Serial I/O ports and interrupt controller;
- Memory card (EPROM and non-volatile RAM with on-board rechargeable battery);
- Special module to control electromagnetic switches (with and without opto coupling);
- Timing unit (e.g. it can be used as a real time clock or to control thyristors or step motors);
- Monochrome display driver;
- A/D converter ("dual slope", resolution: 4 1/2 digits);
- A/D and D/A converters (8 bits);
- Rotational speed controller.

There are further a power supply, as well as thyristor control and safety control modules to prevent overheating.

Several pieces of equipment of a similar kind have been built using these modules to create the control electronics. The same modular system is being used to update various other temperature control systems throughout the Institute. The usual technological units consist of 1-3 zone furnaces with their auxiliary units (gas system, wafer manipulation, injection, etc), each of their cards being run by separate control units and all being linked to one common display with a small keyboard and acoustic warning signal circuit. The system diagram of the temperature control unit of a three zone furnace is shown in *Fig. G-6*.

There are two thermoelements in each of the zones (generally Pt/PtRh 10%), one serving as a the temperature sensor of the control circuit, the other being used by the overheating protection module. The cold junction is a closed thermostat at 50 ^{o}C. The thermovoltage preamplifiers are located there, also. The amplified signal is digitized by a dual slope integrating A/D converter, and it provides efficient noise filtering at the same time. Since the measured signal is subject to artifact rejection, linearization by linear interpolation, cold junction correction and filtering by averaging, the final precision of the computed temperature is limited to 0.1 ^{o}C. The control signal is formed by a parameter optimized DDC algorithm. As the main parameters of the furnace vary considerably with the temperature within the operating range (200 to 1200 ^{o}C), the governing parameters of the digital control program must be varied accordingly. The heating power can be varied by controlling the triacs or thyristors in the primary or secondary coils of the heating transformers. There is also an independent hardware circuit to prevent overheating; it shuts down the furnace if any of the zones is being overheated.

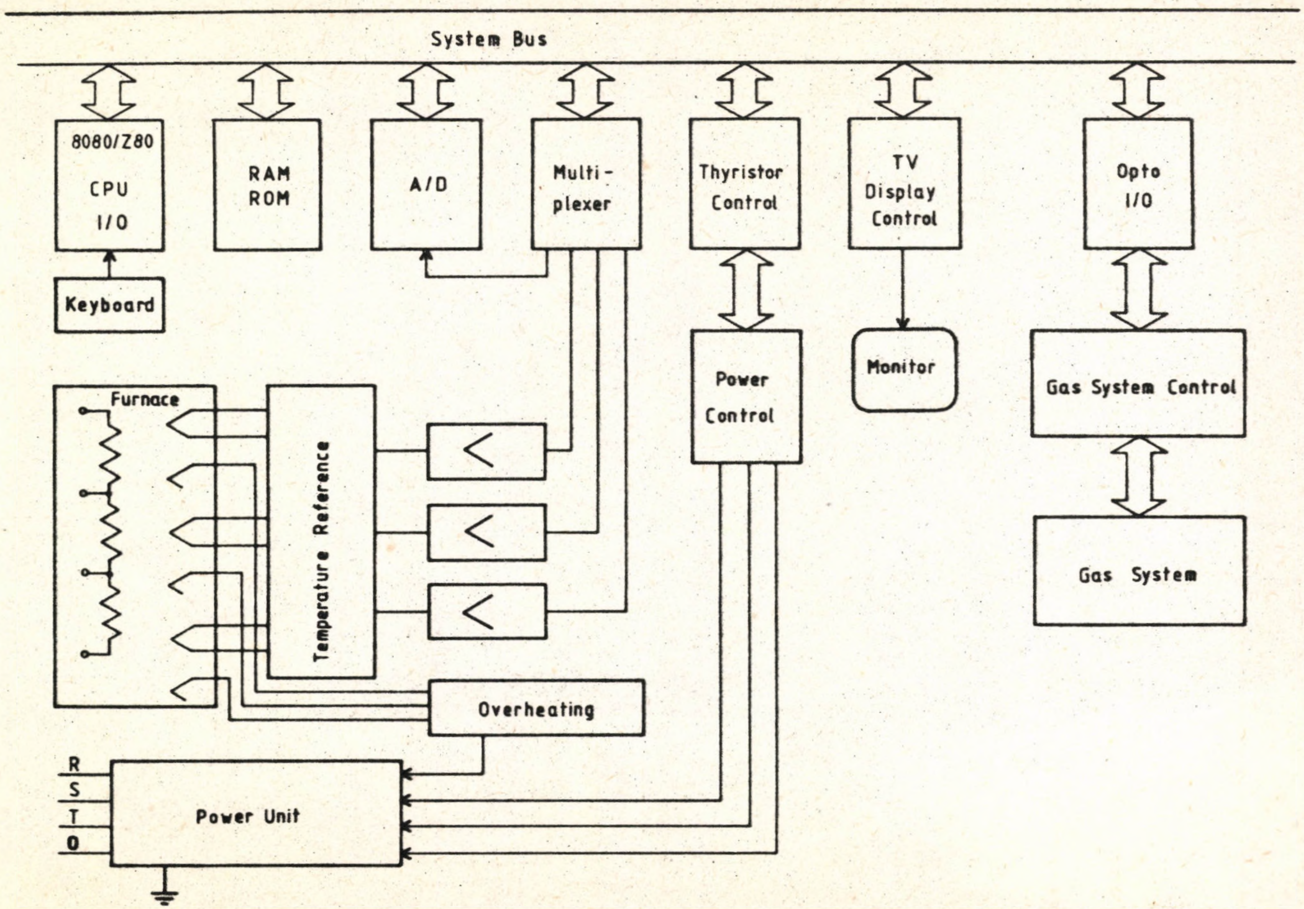

Fig. G-6

System diagram of the temperature control system of a three zone furnace

The sequential control of the electromagnetic valves of the gas system connected to the furnace is done by driving their relays. A relay control program with a maximum of 14 lines can be stored. The lines contain the time delay of the required phase in tenths of seconds and the required state of the valves. Manual control is also possible.

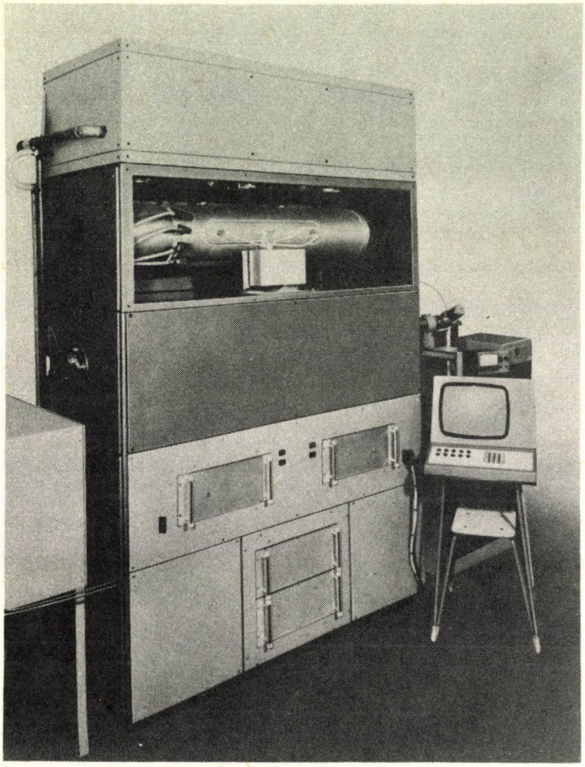

Fig. G-7

Low pressure chemical vapour deposition (LPCVD) furnace

The basis of the software is a modular package of subroutines, elements of which can find application in a broader sense in future designs. The core of the program is a simple real time monitor. The interrupt requests are generated by the A/D converter and by the counter working as a real time clock. Subsequently interrupt subroutines activate the programs that compute and control the temperature, control the valves and execute commands received via the keyboard.

Fig. G-7 shows for example a low pressure chemical vapour deposition furnace that was electronically reconstructed using the electronic modular systems described above.

NEUTRON VELOCITY SELECTOR

Mrs. Tamás Bán, J. Perendi and Gy. Zsigmond

The purpose of the Soviet-Hungarian and French-Hungarian scientific cooperation was the development of a neutron spin echo laboratory for institutes both in Leningrad and in Saclay. Most mechanical units were designed and manufactured in KFKI, among them the neutron velocity selector. In MSzI a novel disc type neutron velocity selector was developed during 1984, in cooperation with scientists and engineers of the Research Institute for Solid State Physics.

The new selector design unites most advantageous features of the selectors known to us (such as the monochrystalline monochromator, the curved aperture and the rotating drum type selectors) without adopting their disadvantages. In this new design the large diameter drum with its specially twisted slots is essentially substituted by a number of appropriately mounted (not equispaced) light metal discs having non absorbent radial slits and radial sections coated with neutron absorbent material (see *Fig. G-8*).

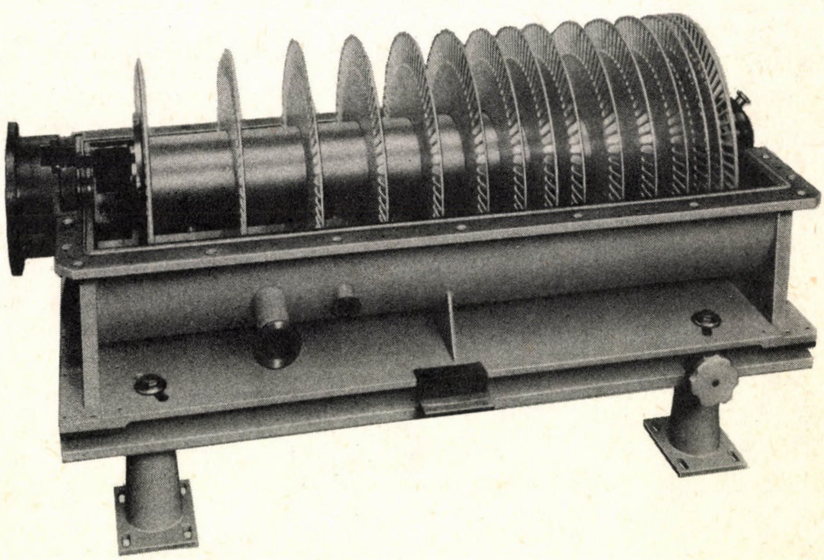

Fig. G-8
Neutron velocity selector

The main advantages gained with the new design are as follows:

- The speed of the rotor can be varied within a wide range (100-7000 r.p.m.), with a relatively low power consumption.
  Result: The selector can be used in a wide wavelength range (2.8-20 Å).
- The large disc diameter ensures a large beam diameter.
  Result: High transmissibility (intensity, 80%).
- There are no undesirable resonances within the range of operation.
  Result: No wavelength ranges are lost.
- The arrangement of the discs can easily be varied according to the requirements of the experiment.
  Result: The neutron beam gained will be free of higher harmonics.

The layout and operation of the neutron velocity selector is simple. It consists of three main parts: the mechanical unit, the D.C. servo motor, and the electronic control unit. The latter ensures the high precision speed control of the rotor and generates the necessary safety interlocking functions *(Fig. G-9)*.

To make operation easy the safety interlock system indicates the correct operation of the individual units with the help of little pilot lamps. Should the value of any observed parameter exceed the preset critical value the corresponding pilot lamp is switched off and subsequently the unit is shut down. Restart is only possible upon removal of the cause of the shutdown and resetting the interlocking system.

At present the neutron velocity selector is working in the Institute in Saclay, France, and current running tests are very promising, confirming previous findings in our Institute *(Fig. G-10)*.

The main technical data

Mains voltage	*220/380 V, +5%-10%, 50 Hz*
Maximum power consumption	*800 VA*
Rotational speed range	*100-7000 r.p.m.*
Rotational speed stability	*± 0.1%*
Long term stability	*± 0.1%/8 hours*

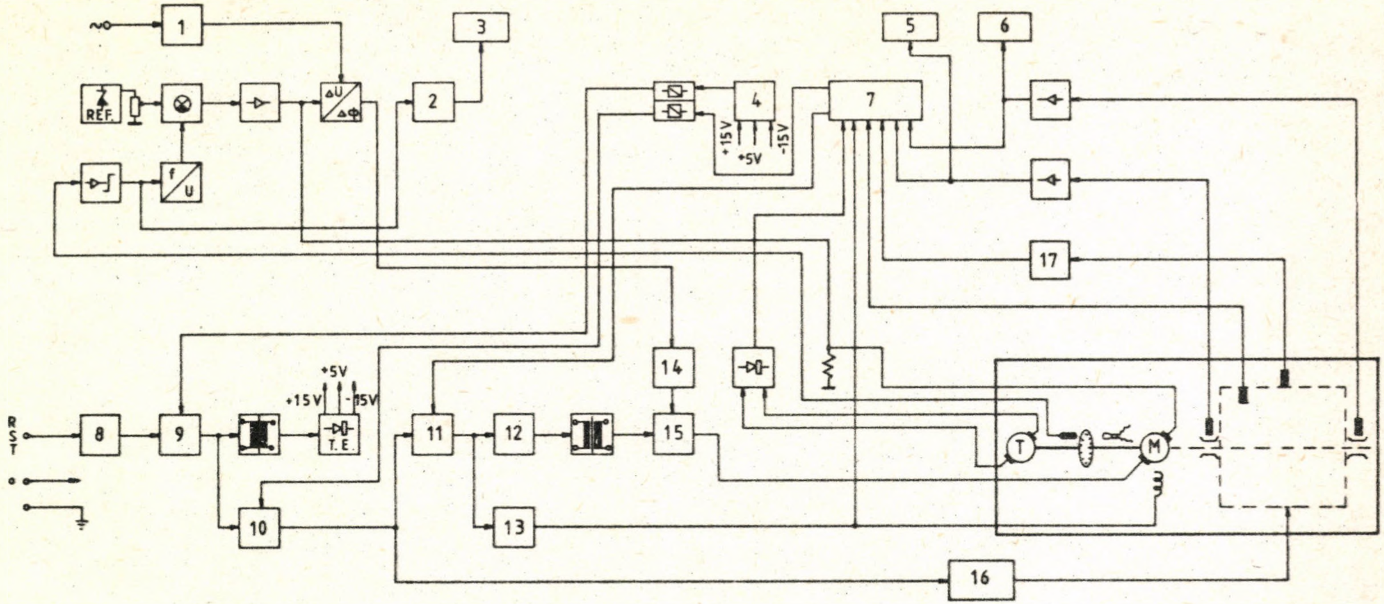

Fig. G-9

Block diagram of the electronic control unit

1. Main synchronizer	*8. Phase monitor*
2. Pulse counter	*9-12. Magnetic switch*
3. R.P.M.	*13. Motor excitation*
4. Power supply monitor	*14. Thyristor control*
5. Bearing temperature	*15. Controlled rectifier*
6. Bearing temperature	*16. Vacuum pump*
7. Level crossing monitor	*17. Vibration pick-up*

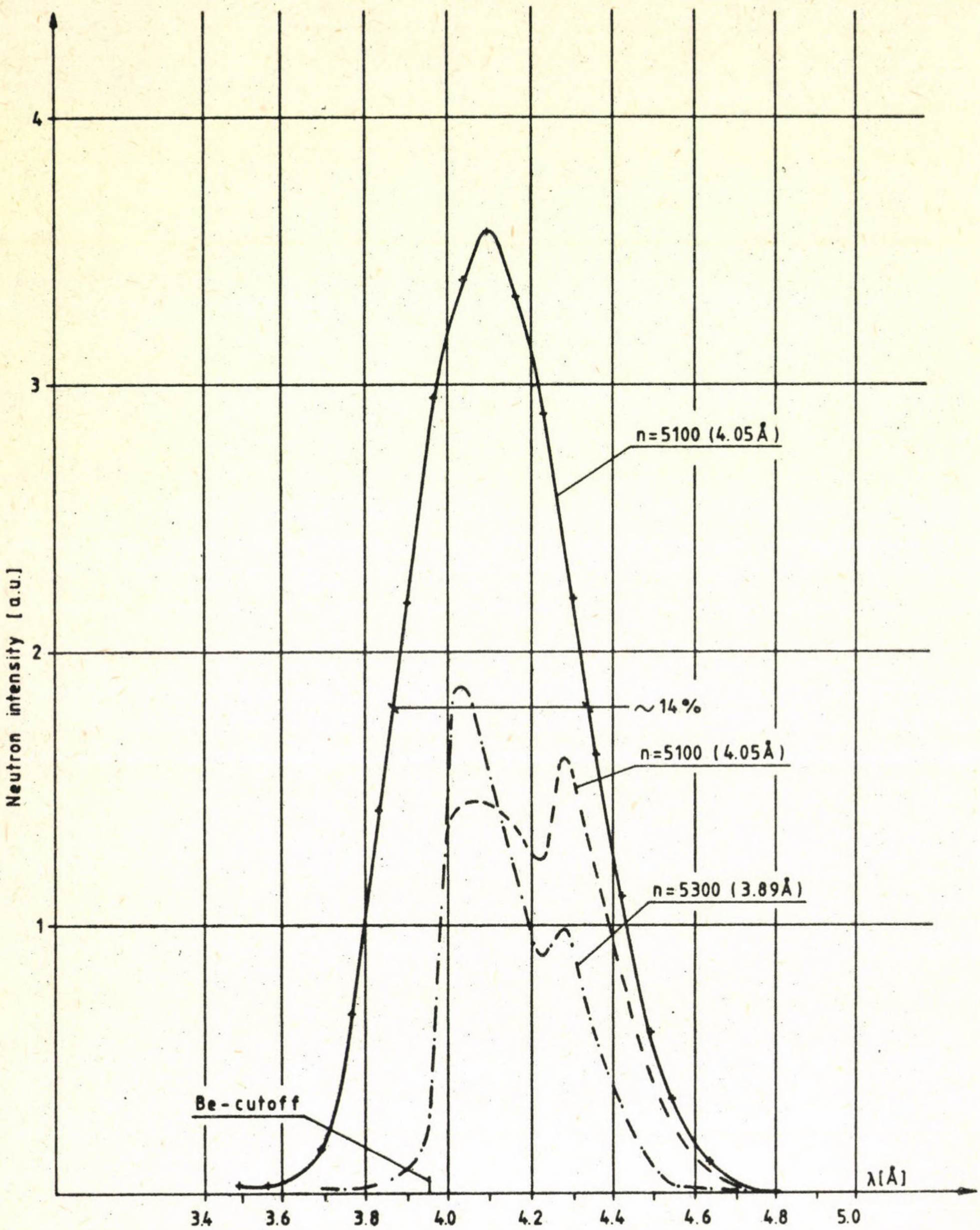

Fig. G-10

Transmission curve of the selector at 4.05 Å and the wavelength calibration by Be-cutoff

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