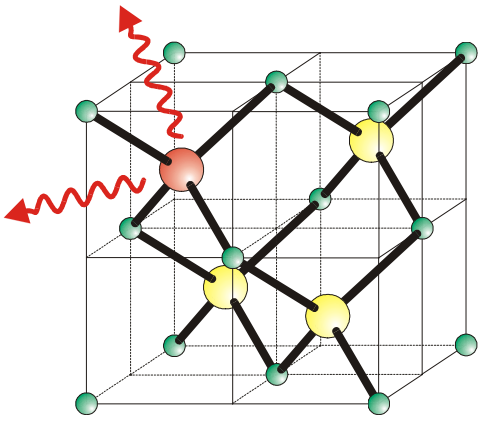
Solid State Physics

at

ISOLDE



January 2002

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for the Solid State Physics Community at ISOLDE

January 2002

Foreword

This document is a condensed presentation of the programme at ISOLDE in the realm of solid state physics with radioactive isotopes.

For reasons of convenience, the corresponding physics programme has been organized into six themes, the first three of which concern semiconductor physics. These themes are:

- Theme 1: Group IV Semiconductors
- Theme 2: III-V Semiconductors
- Theme 3: II-VI Semiconductors
- Theme 4: Surfaces and Interfaces
- Theme 5: Superconductors, Manganites and Opto-electronic oxide materials
- Theme 6: Metals

The document begins with an introduction which emphasises specific characteristics and methods for solid state physics experiments with radioactive isotopes. These are illustrated with a selection of results obtained over the last years in the six themes listed above. In a second section, this introductory part describes the ISOLDE facility and the experimental conditions concerning solid state physics on the CERN site. The next section gives some global data on the community, the size of the programme within ISOLDE, its resources, and its scientific production. The last section provides indications on the perspectives and potential extensions of the physics programme.

The second part of the document describes the recent activities of each of the six themes in relation with the experiments approved by the CERN research board. The presentation of each theme is concluded by a paragraph on short term perspectives.

The third part gives reference to the scientific production by collecting the publications in refereed journals over the past five years.

The fourth part contains the addresses of the groups involved.

I. Introduction

A. Solid State Physics with Radioactive Isotopes

The experiments performed at ISOLDE employ radioactive isotopes as nuclear probe atoms in many different fields of solid state physics: semiconductors, surfaces and interfaces, magnetism, high T_c superconductors, metals, ceramics. One has to keep in mind that the use of radioactive atoms delivered by ISOLDE is only one tool to address specific problems within the different fields, where the application of radioactive isotopes is beneficial or often the only potential technique. In this sense there is no unified solid state physics program at ISOLDE, and the experiments are generally part of often much larger research programs going on in the home laboratories.

The common idea of the scientific activities is directed towards the application of the unique radioactive beams at ISOLDE in the field of solid state physics. This has always been and still is the quest for exploring the potential of the rich variety of different radioactive isotopes for their usage outside of the field of nuclear and atomic physics, which the radioactive ion beams were originally planed for. Along this idea, in different areas of solid state physics, new experimental techniques have evolved which are capable to approach problems that are difficult if not impossible to solve by conventional experimental techniques. Indeed, in many cases, the usage of these radioactive isotopes called for new experimental routes, not been chosen before, in order to enable the investigation of the respective materials, and the developed novel experimental techniques represent the state-of-the-art in the respective fields. Although the research programs proposed and handled by the different groups in the field of solid state physics at ISOLDE do not constitute a unified research program, but rather reflect the scientific interests of the respective groups, synergetic effects have often developed due to the close scientific and experimental collaborations of the different groups at ISOLDE.

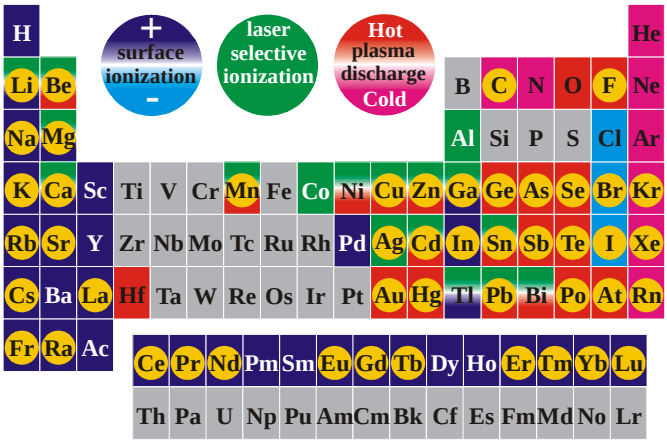


Fig. 1: *The figure shows in colors all elements produced at ISOLDE, by using different types of ion sources, where the most pure ion beams are produced by 'laser selective ionization'. The figure assigns orange circles to the elements where isotopes near stability are currently used in solid state physics experiments at ISOLDE. The EC technique and the 'tracer' techniques (PL, DLTS, Hall effect), where the half-life is the key feature, are the ones who profit most from the variety of elements and isotopes produced at ISOLDE. Almost for each element it is possible to find a suitable isotope.*

Two characteristics of the radioactive ion beams delivered by ISOLDE are of general importance for all experiments in solid state physics: Firstly, their elemental nature, which, e.g., in semiconductors determines their role as constituent atoms or impurities of different nature like donors or acceptors. In this context also the nuclear transmutations (in a decay chain) offer novel experimental approaches unattainable by other means. Secondly, the purity and the intensity of the beams, which boosts the sensitivity of most experiments to orders of magnitude above that of conventional techniques. It can be stated that with respect to both

their variety and quality the radioactive isotope beams available at ISOLDE are worldwide unrivaled. The substantial number of elements, where radioactive isotopes close to stability are available in sufficient intensity exploited in solid state physics at ISOLDE, is shown in Fig. 1. The quality of these beams in terms of purity and intensity exceeds those few available at other facilities in most cases. The implications and consequences of these favorable features for solid state physics, which may not be generally known, will be illustrated briefly here by selected examples and also in the following presentation of the experiments, whereas a comprehensive discussion of the relevance of the experiments within their field of physics is considered beyond the scope of this document and can be found in the corpus of the publications.

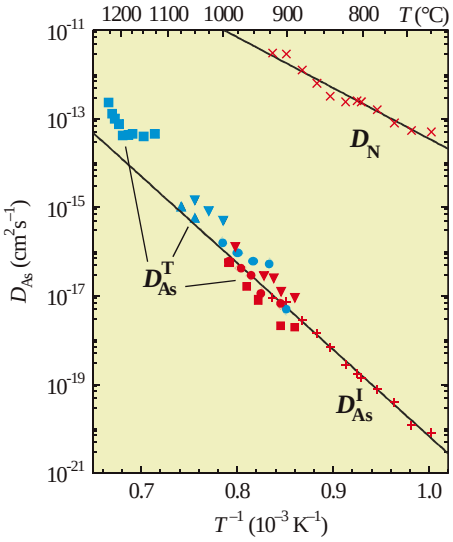


Fig. 2: *Diffusion of As in GaAs: Tracer diffusion coefficients in intrinsic GaAs (D_{As}^T) obtained at ISOLDE (●), from the literature (●,▼) and diffusion coefficients obtained in p-type (▼) and n-type GaAs (■). As diffusion coefficients, D_{As}^I (+), which correspond to the diffusion of interstitial As atoms, and N-diffusion coeffiecients,D_N (×), were obtained from the diffusion of N in GaAs.*

For classical radiotracer diffusion measurements the availability and purity of (short-lived) isotopes at ISOLDE has enlarged the possibilities for studies of self- and impurity-atom diffusivities considerably. For instance, it can be expected that the short-lived ^{31}Si isotope will play an important role in self-diffusion studies in group IV-IV compound semiconductors similar to that of the ^{73}As isotope in III-V compounds, where an unexpected interstitial diffusion mechanism has been revealed for the As self-diffusion in GaAs (Fig. 2). This conclusion was obtained from measurements of both the As-tracer self-diffusion (D_{As}^T) and the N impurity diffusion, from which the As interstitial diffusivity (D_{As}^I) can be deduced as indicated in Fig. 2. These diffusivities are seen to fall on the same line in the Arrhenius plot in Fig. 2, identifying the mechanism.

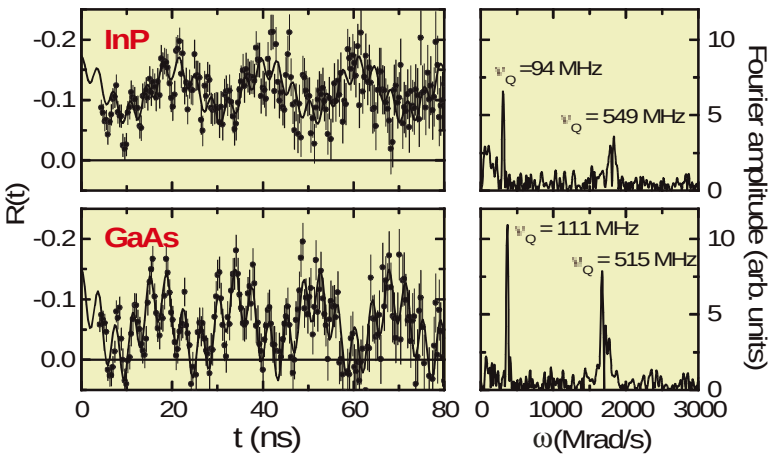


Fig. 3: *PAC signals of unbound H located in the immediate neighborhood of ^{117}In measured at 10 K in InP and GaAs.*

Diffusion data are also obtained from channeling, β-detected nuclear magnetic resonance (NMR), perturbed γ-γ or γ-e$^-$ angular correlation (PAC), and Mössbauer spectroscopy. In the three latter methods a few diffusional jumps are detected within a characteristic time window. Thus H diffusion in III-V semiconductors has been studied by PAC in an intriguing experimental approach. First, the implantation of radioactive ^{117}Cd acceptors combined with an annealing procedure leads to their site-selective incorporation on III-sites. Bound ^{117}Cd-H pairs are then formed with subsequently implanted H, giving rise to an electric field gradient (EFG) at the ^{117}In nucleus in the resulting ^{117}In-H

daughter pairs. The ^{117}In probe atoms are isoelectronic or constituent atoms in the III-V matrices with no or negligible binding to H. Thus a diffusional jump of the H atoms away from the ^{117}In atom during the lifetime of the nuclear state (≈ 100 ns) is detected as a vanishing of the EFG-related PAC signal (Fig. 3).

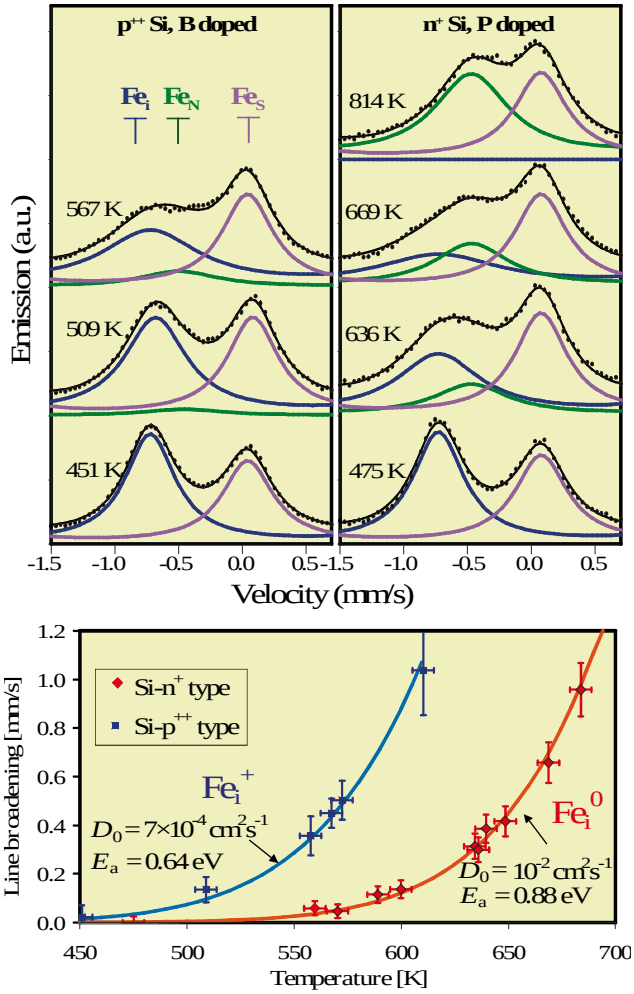
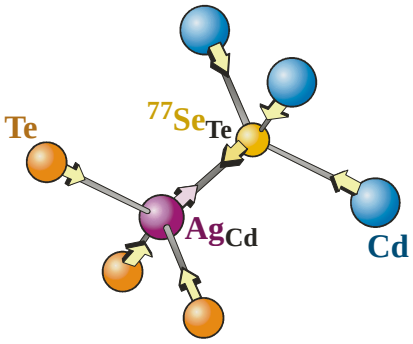


Fig. 4: *^{57}Fe Mössbauer spectra after implantation of ^{57}Mn into differently doped silicon crystals held at the temperatures indicated. The spectral lines from interstitial and substitutional Fe and a new high-temperature line (attributed to the formation of Fe-vacancy pairs) are indicated in the spectra. Note that the line broadening of the interstitial line is similar in p^{++} material at 567 K to that in n^{+} material at 636 K. This different line broadening as a function of temperature is shown in the lower part of the figure and attributed to the two different charge states of interstitial Fe, which thus have different diffusivities.*

In Mössbauer studies of interstitial ^{57}Fe$_i$ in silicon these are first created at diffusion temperatures by the recoil imparted on the ^{57}Fe daughter atoms in the decay of implanted ^{57}Mn parent isotopes. Then, a few diffusional jumps on about the same time scale are detected by the resulting line broadening (Fig. 4), which is directly proportional to the diffusivity. In both types of experiments at the diffusion temperatures the H or Fe$_i$ impurity state is not stable on a minute-to-hour time scale and this (and other complications) has notoriously prevented reliable data to be obtained by conventional techniques for these fast diffusing species. This atomic scale information is of importance also in determining the probe atom lattice location and/or the structure of defect complexes formed with them by means of the probe atom hyperfine interactions. Here the tremendous progress in calculating hyperfine interaction parameters by state-of-the-art theories does now provide a solid ground for structural models. Thus, e.g. the radioactive ^{77}Br and ^{111}Ag provided by ISOLDE enabled studies of donor- and acceptor-type defects on both sublattices of II-VI semiconductors via the measured EFG. Structural models for the experimentally observed defect complexes are tested by means of EFG calculations, performed with the linearized augmented plane wave (LAPW) method in the framework of density functional theory. These kind of calculations yield information about the detailed lattice relaxation and the charge state of the complex in addition to the chemical nature of the involved defects (Fig. 5).

The electronic and optical properties of a semiconductor are not only determined by the chemical nature of a dopant but also by its location in the lattice. For decades, the most straightforward method to locate impurity atoms within a lattice has been the ion beam channeling technique, where an external ion beam (e.g. a He beam with an energy of several MeV) is steered by small angle Rutherford scattering along atomic rows or planes of the

crystal. Using this technique, the detection of impurities is limited to concentrations of at least 10^{18} cm^{-3}. The sensitivity of techniques based on the channeling effect can be improved by several orders of magnitude using radioactive impurity atoms located in the crystal under study. The channeling or blocking effects of the emitted charged particles is then detected along different major lattice directions. For the case of electrons, an enhanced emission yield along a certain lattice direction ('emission channeling', EC) is always the result of an emitting atom residing on or close to the respective lattice rows, which guide the electrons towards the surface. A reduced yield or the absence of an increased yield along a major axis ('blocking') hints at an interstitial site of the emitting atom. The reverse is true for the case of positively charged emitted particles. EC requires the introduction of radioactive atoms by implantation because the channeling effect is maintained only for a certain distance between the emitter and the surface.



	Experiment V_{zz} [10^{21}V/m^2]	Theory V_{zz} [10^{21}V/m^2]	Theory d_{NN} [Å]
$^{77}Se_{Te}$-Li_{Cd}^-	–	–13.5	2.51
$^{77}Se_{Te}$-Cu_{Cd}^-	±5.3(2)	–3.6	2.46
$^{77}Se_{Te}$-Ag_{Cd}^-	±6.7(2)	–6.7	2.64
$^{77}Se_{Te}$-Au_{Cd}^-	±2.6(3)	–1.1	2.64

Fig. 5: *Structural model of a defect complex containing the group I acceptor Ag_{Cd} in CdTe and shown after the decay of the $^{77}Br_{Te}$ donor, with which initially the donor-acceptor pair was formed (left). LAPW calculations, which yield the lattice relaxation (e.g. the Ag-Se distance d_{NN}) and the EFG component V_{zz} at the $^{77}Se_{Te}$ site, show excellent agreement with the experimental V_{zz} values (see table). Since the calculated EFG is sensitive to the charge state of the complex, information about the actual charge state of the defect is obtained.*

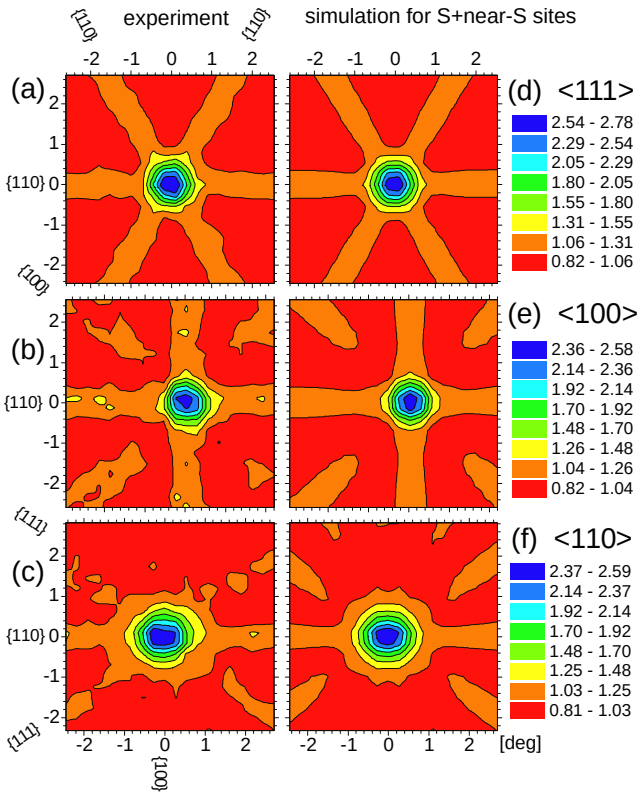


Fig. 6: *Normalised experimental emission yields of the integral b- intensity of ^{67}Cu in the vicinity of <111> (a), <100> (b), and <110> (c) directions in n-Si:As after annealing at 600 °C; panels (d), (e), and (f) show best fits of simulated patterns to the experimental yields, corresponding to 90% of Cu on ideal substitutional sites.*

Along with Fe, Ni, and Co, the element Cu is the most common but unwanted transition metal impurity in silicon devices. It interacts with various dopants and other defects. Positively charged Cu is the fastest known interstitial diffusor in Si. At high temperatures the solid solubility of Cu in Si is the highest among all transition metals but it is negligible at room temperature. As a consequence, Cu shows a strong tendency to react with

various defects and to form precipitates. Using the sensitivity of the EC technique, the first direct determination of the lattice location of Cu in Si became possible (Fig. 6). In summary, the experiments presented so far can be characterized as a class determining basic properties mainly of important impurities in group-IV, III-V, or II-VI based semiconductors such as their lattice location, electronic and vibrational properties, their diffusivity and interactions with other impurities or lattice defects.

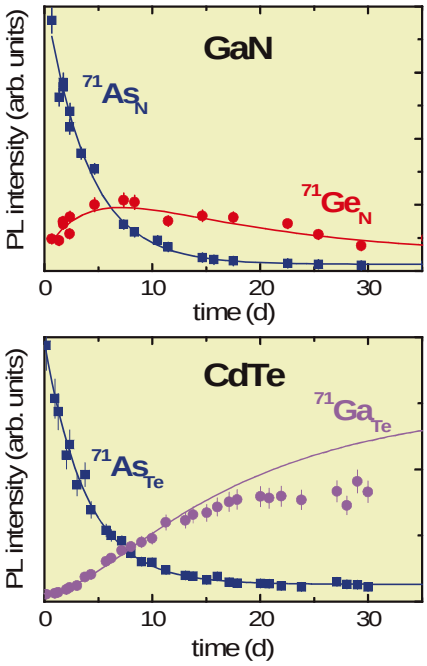


Fig. 7: *Creation of defects by site-selective implantation of ^{71}As into GaN ($^{71}As_N$) and CdTe ($^{71}As_{Te}$) followed by the decay chain $^{71}As \rightarrow ^{71}Ge \rightarrow ^{71}Ga$ and observed by recording the PL intensities as a function of time. Of particular interest are: In GaN, the formation of Ge acceptors ($^{71}Ge_N$) and the absence of the Ga antisite defect ($^{71}Ga_N$); in CdTe, the formation of the shallow acceptor Ga ($^{71}Ga_{Te}$), although Ga usually forms a donor as Ga_{Cd}.*

The presence of such defects/impurities in semiconductors then leads to specific changes of the electrical and optical properties. These can be directly determined by a different class of techniques: capacitance-voltage (C-V), Hall effect, deep-level transient spectroscopy (DLTS), and photoluminescence (PL) measurements. While these techniques are generally very sensitive and provide a detailed mapping of such properties, like deep states in the band gap (DLTS, PL), they are "chemically blind", i.e. cannot easily identify the nature of the impurities/defects causing such properties. This deficiency has been overcome by the application of radioactive isotopes, where the decay of a parent isotope and/or the time-dependent increase of a daughter isotope allows for an unambiguous identification of the origin of an observed time dependent signal. Such studies at ISOLDE have led to the rejection of a considerable number of wrong assignments in the literature on the one hand and to the unequivocal identification of previously known and new centers on the other hand. However, also novel experimental possibilities have been or will be explored, e.g. the controlled creation of specific defects by a site-selective implantation followed by a nuclear transmutation. The implantation of e.g. ^{71}As into GaAs or GaN is known to result in a substitutional incorporation on As or N sites, respectively. In the nuclear decay chain $^{71}As \rightarrow ^{71}Ge \rightarrow ^{71}Ga$ the recoil energies are too small to alter the lattice position, thus first Ge acceptors on As sites and then Ga_{As} or Ga_N anti-site defects are created. By using the characteristic nuclear half-lifes of ^{71}As ($t_{1/2}$ = 65.3 h) and ^{71}Ge ($t_{1/2}$ = 11.2 d), the respective properties of the three different elements can be studied, as was done e.g. by measuring the time dependence of the intensity of the emitted PL lines for GaN and CdTe (Fig. 7). It is obviously attractive to combine the types of experimental classes sketched above for a more comprehensive characterization of defects; this pathway has been pursued to a large extent already for II-VI compounds as presented under theme 3 and will become more important also for other semiconductor systems in the future.

Experiments in metallic systems at ISOLDE are focused on magnetic properties in particular as measured by hyperfine interaction techniques (PAC, nuclear orientation (NO), and Mössbauer spectroscopy). The extreme sensitivity of magnetic hyperfine interactions of PAC probe atoms is exploited in studies of magnetic interactions at surfaces and interfaces. Here the isobaric purity of the ISOLDE beams is of utmost importance as well as the

possibility to use different probe atoms on the same systems for systematic studies of, e.g. sp-elements as ad-atoms on a nickel surface, where detailed theoretical predictions could be tested critically. Recently, within epitaxially grown Pd layers on nickel surfaces Pd or Cd PAC probe atoms were positioned in a controlled way at different distances from the interface. The different probe atom locations in such experiments are illustrated in Fig. 8. The measured static magnetic hyperfine interactions revealed a ferromagnetic ordering of the Pd layers of rather complex nature as evidenced by Pd magnetic hyperfine field distributions. By contrast, discrete hyperfine fields were measured for Cd impurities and attributed to specific lattice locations.

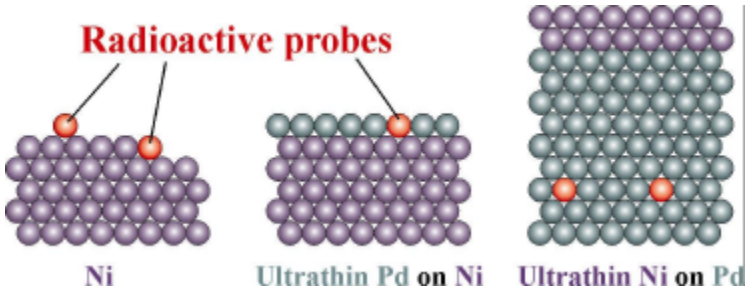


Fig. 8: *The icons symbolize the three pioneering experiments performed with ASPIC. Left: Radioactive probe atoms were positioned at different surface structures of Ni (e.g., terraces, steps kinks) and the magnetic hyperfine fields were measured with an unsurpassed structural resolution. Center: The 'ferromagnetic' behavior of ultrathin Pd grown on Ni, was investigated with different probes. Right: Magnetic properties in Pd, induced by a coverage of ultrathin Ni on Pd, were investigated in dependence of the distance from the Ni/Pd interface.*

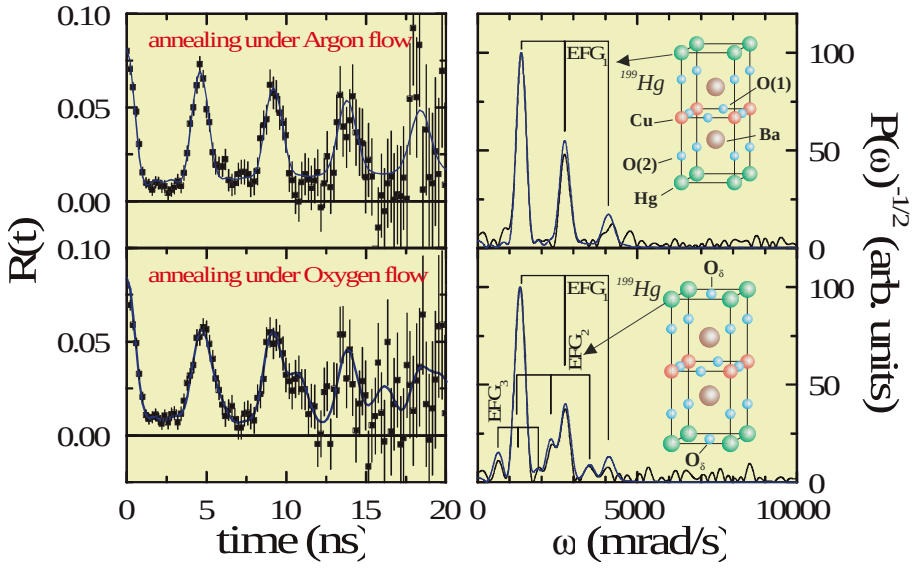


Fig. 9: *^{199}Hg PAC time spectra, R(t), measured on Hg1201 (n=1): (left-top) measured under Argon flow (undoped material) and (left bottom) measured under oxygen flow (oxygen doped material). Right pictures show the corresponding Fourier transforms of the R(t) functions. In the R(t) and the Fourier spectra the blue lines represent the PAC fit function and the Fourier transform of the fit function, respectively. While EFG_2 could be assigned, from first principle calculations of the electronic density, to oxygen sitting in the centre of the Hg channel, EFG_3 is due to a still unknown oxygen related defect.*

Recently, studies of oxides, predominantly by PAC and EC techniques, have been added to the spectrum of solid state physics at ISOLDE. These comprise high T_C superconductors,

manganites, and optoelectronic oxide materials. The application of the novel short-lived ^{199m}Hg PAC probe atoms ($T_{1/2}$ = 43 min) to high T_C oxides and to O_δ (oxygen) doped $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ in particular, has been very rewarding. It could be shown that the O_δ^{2-} dopants occupy interstitial sites in the Hg planes, giving rise to two different EFGs at the Hg site (which, at the same time, are different from that present from the tetragonal lattice structure in undoped material, Fig. 9). One of these EFGs, *EFG_2*, as well as that for undoped material, *EFG_1*, are found in very good agreement with values calculated by ab-initio local density approximation techniques, thereby identifying the local defect structure. Further, more comprehensive studies have been initiated as outlined under Theme 5.

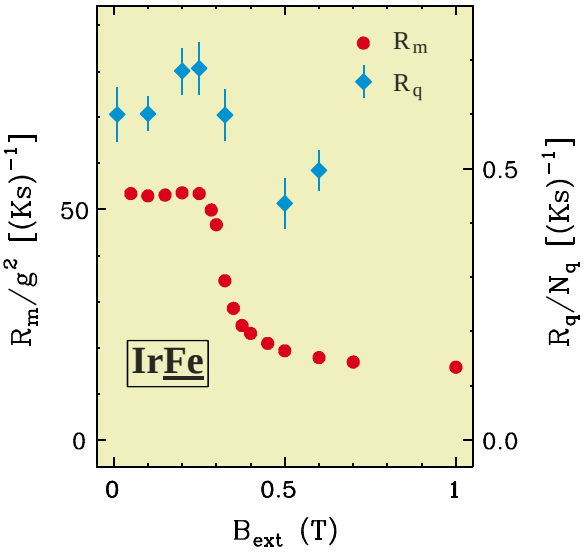


Fig. 10: *The reduced magnetic and electric quadrupolar relaxation rates of Ir in Fe as a function of B_{ext} applied along [100]. Due to the choice of the ordinate scales the relative magnitude of the rates in the figure reflects the situation for ^{189}Ir. (cf. Theme 6).*

In NO experiments on implanted 5d impurities (Os, Re, Ir, Au, Pt, Hg) in magnetic 3d matrices, very subtle details of the probe atom hyperfine interactions are measured, e.g. the presence of an electric field gradient on lattice sites of cubic symmetry due to the spin-orbit interaction. These efgs and their inhomogeneous broadening were shown to depend on the angle between the magnetization and the crystal directions in cubic Fe and Ni matrices. In hcp Co the spin-orbit induced efg was found to be either zero or relatively large. A theoretical understanding of the observed effects is still missing. This applies also to the measured quadrupolar contribution to the nuclear spin lattice relaxation for Ir in Fe. This measurement became possible by an intriguing experimental approach, where two Ir isotopes (186 and 189), with strongly different quadrupole-to-magnetic moment ratios, were implanted into the same sample. Thus the magnetic relaxation rates of orbital and non-orbital nature could be separated for the first time and the latter was found to be dominant - contrary to theoretical results (Fig. 10).

B. Facility and Instrumentation

At the European Organization for Nuclear Research CERN, proton beams are used for a variety of experiments in elementary particle physics, e.g. at the Proton Synchrotron and the Super Proton Synchrotron. These accelerators are fed with protons by the booster accelerator PSB (energy 1.0 or 1.4 GeV, average current 2 μA). These energies are suitable for the production of radioactive ion beams exploiting the Isotope Separation On-Line principle at ISOLDE. Radioactive isotopes are produced in a thick target by fission, spallation or fragmentation, diffuse out and are ionized via/by a plasma, laser or surface ionization ion source (see HRS and GPS Target in Fig. 1). The singly charged ions are then accelerated to an energy of 60 keV, mass separated and available for the experiments at different beamlines (Fig. 1). This way, exotic nuclear probes, i.e. isotopes which cannot be produced in a classical fashion or that are to shortlived for usage off-line after production, are available carrier-free as an isotopically clean beam. They can be collected in a beam stopper for the study of nuclear

properties, manipulated in an electromagnetic trap, or implanted into any solid material to be studied.

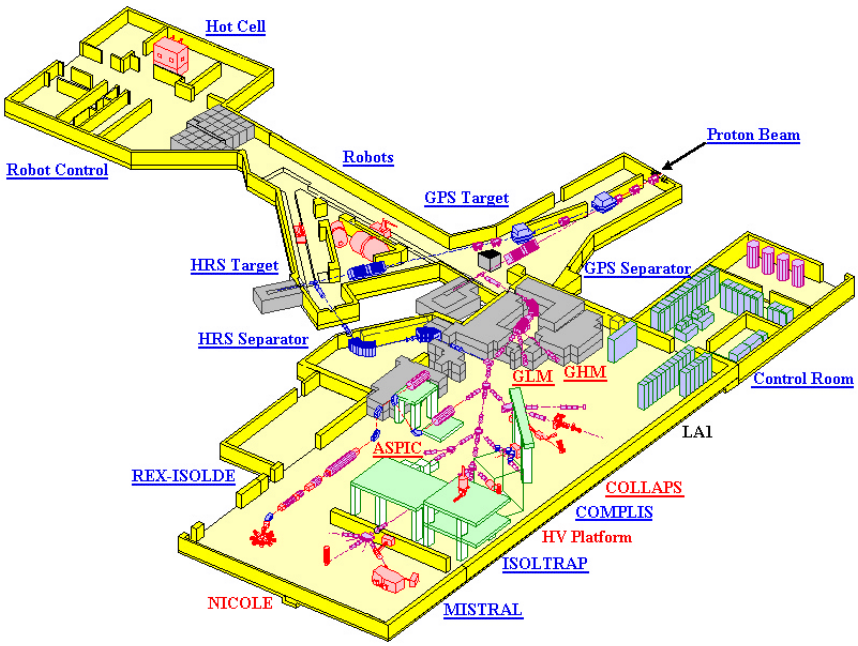


Fig. 1: *Layout of the ISOLDE facility. Solid state physics mainly uses the General Purpose Separator GPS (violet). The experiments are carried out at the GLM and GHM beam lines and the setups of COLLAPS, the HV platform, NICOLE and ASPIC.*

The beam current (up to nanoamperes) and the purity of the beam of a specific isotope (600 isotopes of some 70 elements are available so far) is optimized by choosing the appropriate target/ion source combination. Up to 40 target/ion source units can be used over the experimental period of a year. In this way, several experiments share the beams available from a certain target within one week.

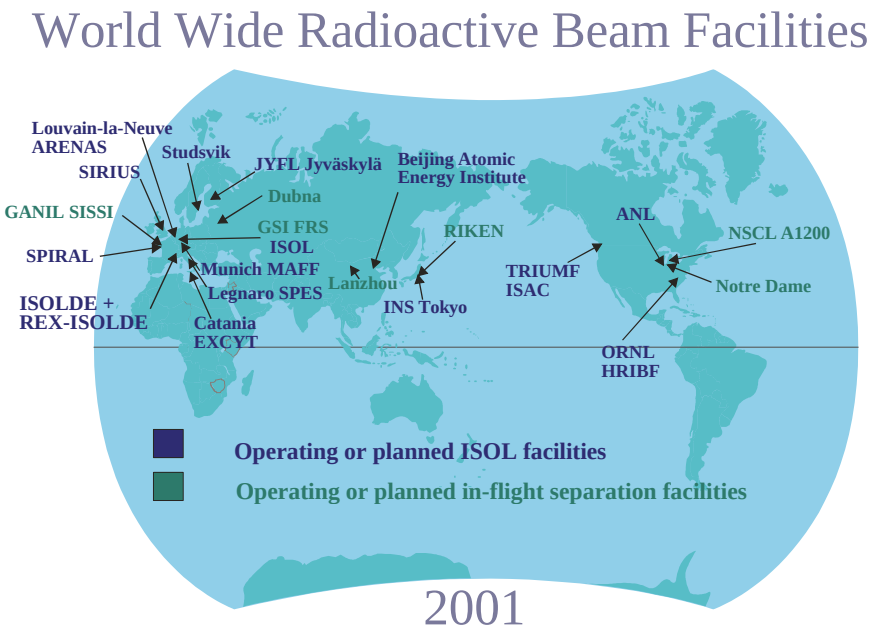


Fig. 2: *World map showing operating or planned ISOL and in-flight separation facilities.*

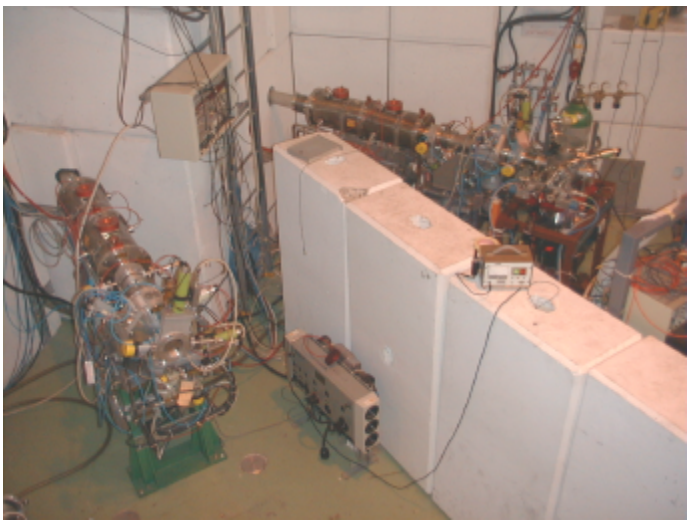


Fig. 3: *The GLM beam line on the left is free while a collection chamber is connected to GHM (right).*

Physics at ISOLDE is pursued in several directions such as particle and astrophysics, biology/medicine, atomic physics, weak interaction/nuclear physics and solid state physics. The existence of the diverse solid state physics programs is a consequence of the exceptional quality of the radioactive beams delivered at ISOLDE. The ion beams are isotopically pure which gives the experimentalist the possibility to take full advantage of the fact, that nuclear methods need only a rather small number of probe atoms compared to classical spectroscopy. Furthermore, experimentalists are enabled to exploit isotopes of various elements under exactly the same experimental conditions. The number of isotopes available at ISOLDE for hyperfine interaction studies is about a factor five larger than at the home institutes. For the emission channeling technique, working with 2-dimensional electron detectors, radiotracer diffusion studies, and the novel 'tracer' techniques like photoluminescence spectroscopy, where the half-life of the isotope is the key feature, for almost each element it is possible to find a suitable isotope, and there still exists many elements to be tested and applied. High yields allow dose tuning and systematic studies on a sufficiently large number of samples during a single beam time. These characteristics underline the outstanding position of ISOLDE among the ISOL facilities operating worldwide (Fig. 2).

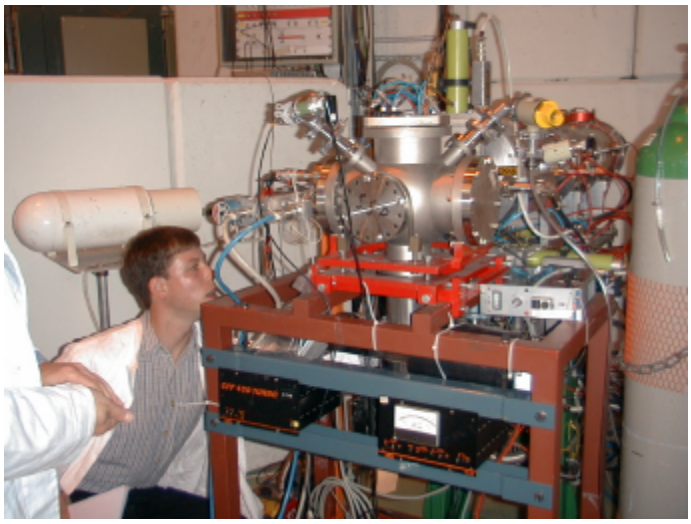


Fig. 4: *'Solid State Physics Chamber' operated at the GHM beam line. Both sample holder and collimator are introduced from the top.*

The radioactive ion beams that are used for both off-line and on-line experiments in solid state physics are mainly delivered by the General Purpose Separator (GPS) (Fig. 1). The main switchyard behind the separator magnet directs beams of different masses to three beam lines in parallel. For the off-line experiments, implantations can be carried out at the two short beam lines GLM and GHM (Fig. 3). Two collection chambers are available permanently at ISOLDE. Up to ten samples can be mounted at once and implanted without breaking the vacuum. While the 'Solid State Physics Chamber' (Fig. 4) is more versatile because of exchangeable collimator plates and optional sample heating, the 'New Collection Point' (Fig. 5) is especially suitable for the collection of high activities because of its lead shielding and the sample transfer system. Some experiments use dedicated implantation chambers that meet

their specific needs. Whenever the mass difference of the isotopes permits, different experiments are carried out in parallel at the GLM and GHM beam lines. A postacceleration of the ions to an energy of 260 keV is possible on the High Voltage Platform further downstream the beam line (Fig. 1).

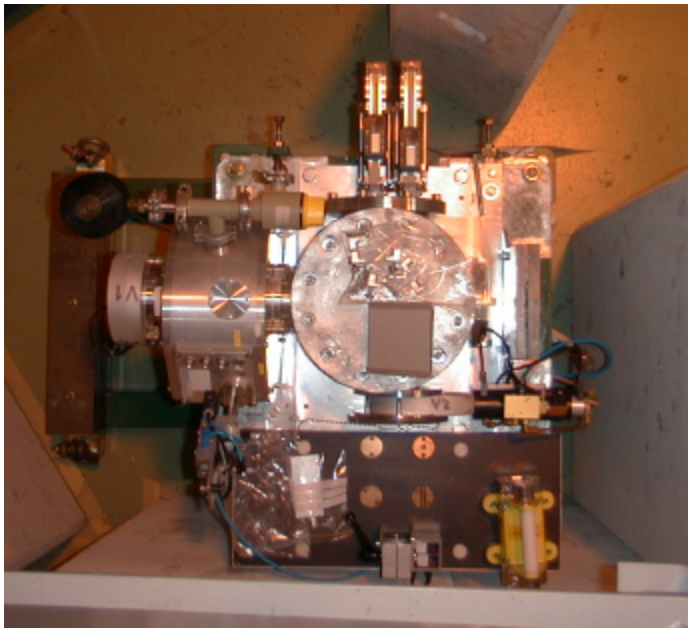


Fig. 5: *Top view of the 'New Collection Point' as disconnected from a beam line. The connection to a beam line is on the left and the sample holder is introduced from the bottom of the picture. Sample holders can be taken out of the chamber directly into the shielded transport container (bottom right, yellow).*

For on-line experiments, the GHM/GLM beam lines are used if the installations for the experiments are temporary ones. Experiments that require more complex setups for several years like COLLAPS (which produces polarized ion beams by laser polarization used by β-NMR) or NICOLE (Nuclear Orientation experiments at temperatures below 1 K) are installed permanently at dedicated beam-lines (Fig. 1). One beam-line is capable to host experiments that require ultra high vacuum like ASPIC (surface and interface experiments) (Figs. 1 and 6).

A 'Solid State Physics Laboratory' (Fig. 7) exists nearby the ISOLDE hall where sample preparation and treatments are done during beam times. The laboratory is equipped with devices serving basic needs for experiments in solid state physics and life sciences (furnaces, exhausts etc.) and the running costs are covered by the German BMBF.

Space in the ISODLE hall required for the temporarily set-up of spectrometers has decreased drastically within the last years. A planned extension of the 'Solid State Physics Laboratory' will improve this situation in the future. This extension is required for the permant installation at ISOLDE of a photoluminescence spectrometer which has been funded by the BMBF. This new laboratory with the permanently installed photoluminescence spectrometer and space for temporarily installed additional equipment like DLTS spectrometers opens the possibility to use isotopes in solid state physics experiments which are too short-lived to be transported to the respective home laboratories.

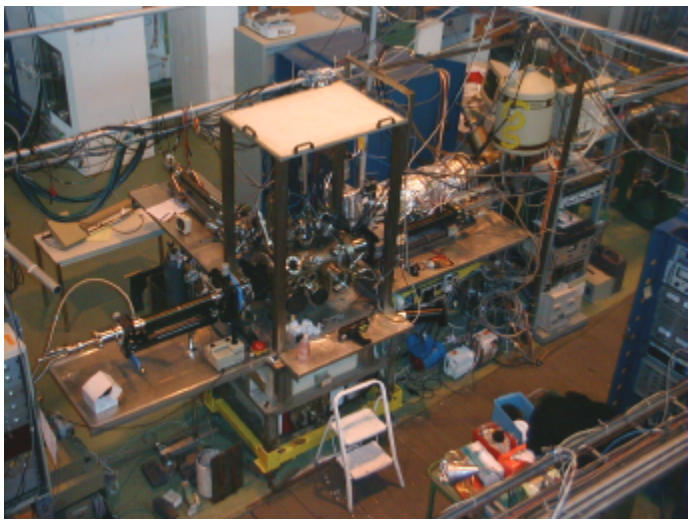


Fig. 6: *ASPIC setup for surface and interface science installed at the UHV beam line (from top right). Three manipulators are connected to the main chamber.*

There exists an 'ISOLDE off-line Laboratory' that houses spectrometers, which are shared among the users and are kept permanently on site. The setups consist of one 6-detector γ-γ PAC spectrometer from the University of Leipzig (mainly financed by the BMBF), one e^--γ PAC spectrometer from the University of Lisbon and three emission channeling setups (financed by CFNUL-Lisbon, ITN-Sacavém and IKS–Leuven) (Fig. 8). Experiments using long lived isotopes with half-lives from a few hours up to several months are running during the full year, also during accelerator shutdowns.

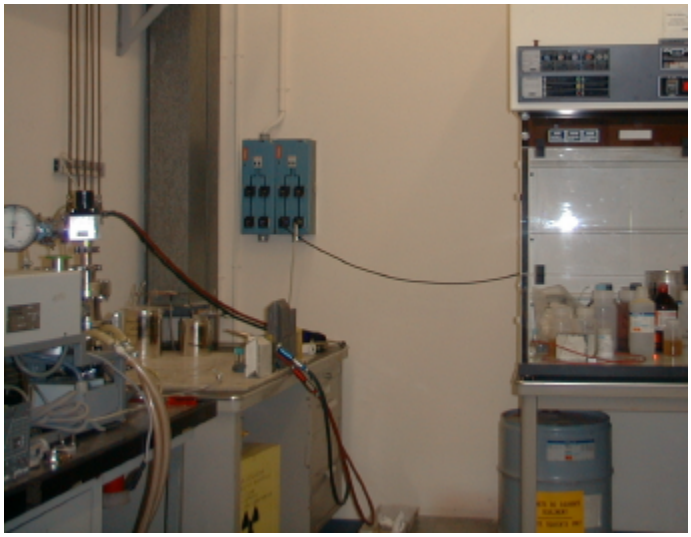


Fig. 7: *In the 'Solid State Physics Laboratory' behind the ISOLDE hall sample preparation is carried out. The photograph shows the vacuum pump stand and the hydrogen burner for ampoule sealing and an exhaust serving chemical preparations.*

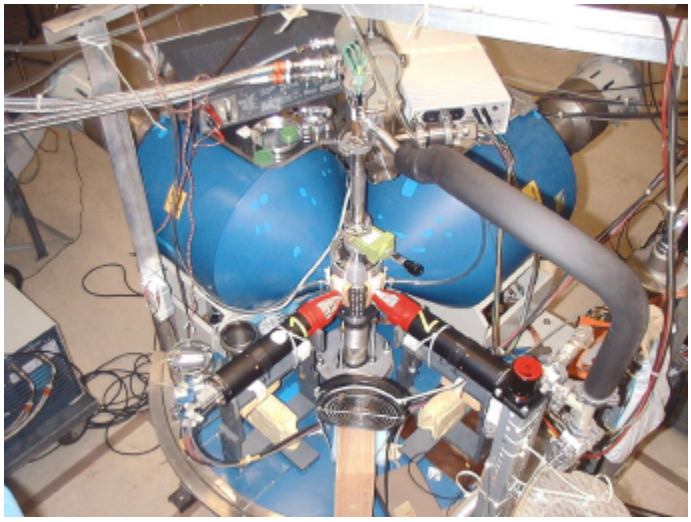


Fig. 8: *Left: Top view of the e^--g PAC spectrometer. The blue elements are magnetic lenses for detection of conversion electrons. The two black cylinders are gamma detectors equipped with BaF_2 scintillators. The samples are mounted in the center, and can be measured from 30K up to 920K. Right: One of three emission channeling setups equipped with the PAD Si electron detector and readout systems developed at CERN. Presently samples can be annealed in situ, up to 1170K.*

C. Statistical Data and Financial Contributions

During the years 1998 to 2001, in the yearly average 15 solid state physics experiments, corresponding to 38% of the experiments, have used 54 shifts (1 shift = 8 hours) of radioactive beam, i.e. 22 % of the total number of shifts delivered. The evolution of the number of shifts used and accepted experiments running per year is shown in Fig. 1.

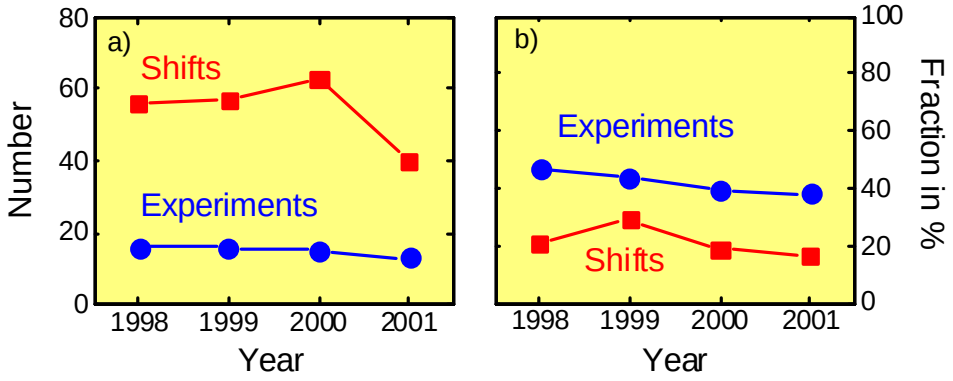


Fig. 1: *Numbers of solid state physics experiments (circles) and the radioactive beam time (squares) used within the years 1998 and 2001 in shifts (1 shift = 8 hours). a) Absolute numbers. b) Percentage with respect to total numbers including all ISOLDE experiments.*

Statistics on collaborations and scientific production

The following total numbers have been extracted from the chapters III. "Scientific Output" and IV. "Administrative Data" in order to illustrate the vitality of the collaborations and the research.

Participating institutes	63
Participating countries	16
Publications (last 5 years)	181
PhD thesis (last 5 years)	27
Invited talks and schools (last 5 years)	94
Conference contributions (last 2 years)	113

Funding agencies

In addition to the financial contributions of the respective home institutes, funding by the external agencies listed below is essential for the success of the physics program:

- Bundesministerium für Bildung und Forschung, BMBF (Germany)
- Danish Science Research Council: Instrument Center for CERN, ICE (Denmark)
- Deutscher Akademisher Austauschdienst, DAAD (Germany)
- Deutsche Forschungsgemeinschaft, DFG (Germany)
- European Commission:
    - European research network RENiBEl 'Rare Earth doped Nitrides for high Brightness Electroluminescent emitters'

  - European Network on Defect Engineering of Advanced Semiconductor Devices
  - Access to Research Infrastructures
- Fonds voor Wetenschappelijk Onderzoek Vlaanderen, FWO (Belgium)
- Fundaçao para Ciência e a Tecnologia, FCT (Portugal)
- German Israelian Foundation, GIF (Germany, Israel)
- Material science evaluation committee of the Federal State of Nordrhein-Westfalen (Germany)

Budget

The following table contains the investments carried out by the solid state physics experiments running at ISOLDE, both on site at CERN and at the home institutes. The total number of positions refers to full man-years/year:

Investments	at CERN	1900 k€
	at home institutes	2700 k€
Maintenance and Operation	at CERN	150 k€/year
	at home institutes	650 k€/year
Positions (100%)	at CERN	1
	at home institutes	53

Additionally, the German community runs (for the years 2001-2004) a common project funded by the BMBF including investments of 250 k€ (Setup of a photoluminescence spectrometer at CERN and maintenance of the solid state physics lab at CERN), 50 k€ travelling expenses and the full position of the ‘Solid State Physics Coordinator’ permanently present at CERN. This person acts as contact person between CERN and the community.

D. Perspectives

In the field of semiconductor technology, the presently dominating silicon device technology is expected to prevail for the next decades; challenges for future technology developments (structural dimensions below 100 nm, increasing wafer diameters, integration of 10^8 elements in one processor) have been identified in the *International Technology Roadmap for Semiconductors* (http://public.itrs.net/). Of concern are, e.g., metal impurity concentrations both in the starting material and incorporated during processing, which have to be controlled to concentrations below 10^{10} cm^{-3}. This is 2-3 orders of magnitude below present standards, where the concentrations often are above thermal equilibrium solid solubility limits. Many of such impurities have been and will be studied at ISOLDE by DLTS, PL, Hall effect, EC, PAC and ME. These are among the very few experimental techniques, which reach the necessary sensitivity and give atomic-scale information on such defects. The results obtained so far suggest two general conclusions: Firstly, the important physical processes change with concentration and, secondly, new non-equilibrium processes are induced under ion implantation conditions. Obviously, the prospects at ISOLDE are extremely favorable to explore further this new area both in terms of a large variety of methods and of probe atoms. In particular, this enables *systematic* studies, which appear necessary to identify the decisive physical processes.

A similar statement can be made for the class of III-V and II-VI compound semiconductors, where present technologies often employ metal atoms in device fabrication, e.g. Fe and other 3d metals to obtain semi-insulating III-V compounds, as well as being used in the growth of synthetic diamonds. For compound semiconductors it has been shown that ion implantation of radioactive isotopes furthermore allows to incorporate via transmutation probe elements on specific lattice sites, which cannot be populated by direct implantation of the daughter atoms. Again, such studies promise to contribute to a better understanding of the often rather complex physical phenomena associated with defects.

An emerging new class of semiconductors are IV-IV compounds like SiGe which are proposed to have a direct band-gap, in contrast to pure Si or Ge. High-speed SiGe devices (> 5 GHz) are competing already now with devices based on GaAs or GaAlAs. Using SiGe instead of III-V semiconductors, the existing and highly developed Si technology can be used for doping and structuring.

Beyond these possibilities for studies of well-established semiconducting materials at ISOLDE, the prospects of the developed techniques show up a potential for addressing specific problems related to the production, doping or the properties of novel materials, which currently appear on the horizon as possible future alternatives.

Although GaN has been the material of choice for short wavelength optoelectronic devices (LED, laser diodes) in recent years, a recent report on laser action in ZnO has opened up a major new technology field. ZnO has a direct band gap of 3.5 eV similar to GaN. In contrast to GaN which can only be produced by epitaxial procedures, bulk ZnO crystals of good quality can now be produced; but, at the same time, ZnO is still one of the most poorly understood materials with respect to impurities, defects, and associated energy levels. For example, as-grown ZnO is intrinsically n-type, and general agreement as to the chemical identity of the dominant donor impurity (interstitial Zn, oxygen vacancies, or hydrogen) is not yet established. Therefore, it is still difficult to produce p-type material in a reproducible way, and this remains an important problem regarding further technological development, i.e. building diodes. As in the case of donors, the identity of the acceptors found in as-produced ZnO is not yet shown.

Magnetic semiconductors, e.g. II-VI and III-V semiconductors containing Mn as magnetic atoms, have very attractive properties for applications in layered spin-electronic devices. Such devices became increasingly important in the last years but there are many open questions concerning a microscopic description of the magnetic coupling in these substances. Using PAC, ME, and EC one gets the possibility to answer questions like lattice position, doping characteristics, thermal behavior and hyperfine fields of doping atoms. Especially, the magnetic hyperfine interaction of implanted radioactive impurities can be easily inspected.

In semiconducting heterogeneous structures as well as in semiconductor nanocrystals, where the reduced size (‘nano physics’) reveals new optical and electronic properties (e.g. quantum dots), the radioactive methods offer the local tools of hyperfine interaction techniques (PAC, Mössbauer effect), as well as the possibility of using spatial (micro-beam) and time resolved photoluminescence in combination with radioactive dopants.

Most of today’s electronic devices utilize the properties of inorganic materials in order to satisfy a particular requirement. However, organic materials potentially offer an increased versatility in device design since their molecular and bulk structure can often be tailored to produce a material possessing specific functional properties (molecular electronics). Examples are the ability of doubling the frequency of laser light (non-linear optics) or of binding gas molecules, such as ammonia or nitrogen dioxide, and as a result to change their own electrical or optical properties (sensors). The extreme sensitivity of spectroscopic

techniques based on the use of radioactive probe atoms could help to get new insights regarding the processes in these materials, e.g. structural properties or electron transport. In particular, the new field of bioelectronics is concerned with the study of the interface between biological and (conventional) electronic systems, particularly at or below the μm-scale. Techniques like PAC and ME with their sensitivity on an atomic scale could be envisaged to study the properties of these interfaces.

As far as ceramic materials are concerned with their much more complex structures and behaviors than semiconductors, the problems addressed in superconductors as well in manganites are specific for each compound. On the other hand, current activities in the area of optical circuits, wave-guides and optical storage systems are promoting crystalline oxides and ceramic materials as relevant media for applications. The possibility of transferring/applying the ion implantation technology, a common method for tuning properties in semiconductors, to these materials would be of great interest once integration is needed. In this domain the possibilities of using radioactive isotopes are by far not exploited yet, cf. the example of the recent industrial interest in the EC technique to look for the lattice site location of Cu in KLTN.

The new technical developments will include the setup of a photoluminescence spectrometer at ISOLDE. It will enable studies of semiconductors with very different band gap energies, from Ge up to GaN, SiC, and ZnO, by using an appropriate set of lasers and detectors for excitation and detection, respectively. This spectrometer together with a ‘semiconductor lab’ at ISOLDE will allow to use short lived radioactive isotopes with half-lives down to 1 hour in semiconductor physics. In addition, developments of highly sensitive 2-dimensional electron detectors for EC measurements will enhance the maximum possible count rate to above 10 kHz. This is a prerequisite for carrying out EC studies on-line with short-lived isotopes. At the same time, the low energy limit of detection is expected to be decreased to 10 keV. The lower energy threshold will open the possibility to study also low-energy electron emitters, as they are used, e.g., in conversion electron Mössbauer spectroscopy, for studies of structures located near the crystal surface or in the analysis of very thin crystalline layers. In this way, systems can be studied under identical conditions both by EC and ME.

New perspectives will open at ISOLDE with the availability of intense high energetic radioactive ion beams. Due to the present beam energy of 60 keV (260 keV using the high-voltage platform) the probe atoms are localized 10-100 nm below the surface after implantation. For studies of dopants and defects in semiconductors, higher energies are often desirable in order to deposit the radioactive isotopes deeper in the bulk, that is, outside the range of surface related defects and the space charge region. By varying the energy of the ions in the 0.1-10 MeV range, homogeneous depth profiles can be produced with a much lower dopant concentration. Phenomena that are highly sensitive to the influence of the Fermi level (i.e. the doping level), such as passivation mechanisms due to the trapping of mobile impurities or defects, can be studied in this way. The close vicinity of the surface to the implanted region is also a strong limiting factor when comparing data from different techniques, which are sensitive to different depths. The high-energy beams will also allow to reach a specific layer in a multi-layered structure.

In summary, the objectives of solid state physics at ISOLDE have expanded pronouncedly during the last decade. The number of fields of physics have increased, where the application of radioactive isotopes has been demonstrated to have a great potential. This has to a large extent become possible by the development of novel, innovative experimental techniques both for the production of radioactive isotopes and their applications. It is very regrettable that in recent years the solid state physics activity at ISOLDE, when measured in terms of beam time

for solid state physics experiments has been reduced (see Fig. 1 in section I.C), mainly owing to the problems with the GPS in 2001. In this context we would like to emphasize the necessity for most experiments to obtain beam time more often than once p.a. in order to achieve a healthy experimental program. In particular, it is crucial for a timely publication of the results and mandatory for the participation of master and Ph.D. students in the experiments, since these young physicists have strict time constraints for the completion of their theses. As sketched above, the prospects for new physics developments at ISOLDE are bright. It should be also noted that this evaluation of the potential for interesting research is universally shared as testified by the fact that, at all the recently commissioned or future radioactive ion beam facilities, solid state physics has become an integral part of the planned experimental program.

We are therefore deeply concerned that decisions taken by CERN to cope with its present financial problems might reduce significantly the beam time allocated to non LHC programs. We believe that this would generate a waste of the unique resources developed at ISOLDE by the CERN and outside physicists and engineers. It would not only hinder the activity of solid state physics community but also weaken the present leadership position of CERN in this particular domain.

II. Scientific Program

Foreword

This part of the documents describes the recent scientific activity within the six themes. Each theme is organized in chapters according to classes of studies. Associated to each class are the CERN labels of the concerned approved experiments. Depending on their status in the decision process line they are called ISxxx or Pxxx where xxx is a three digit number. These experiments are more extensively described in the papers listed in the third part of this document and in documents accessible via the CERN site.

For instance, to reach the proposal of experiment IS395 one goes to ISOLDE's home page at http://cern.ch/isolde, selects **Experiments** from the Main Contents and finds aside IS395 the proposal number **P139** which is linked to the original proposal. The link **Publications** at ISOLDE's homepage Main Contents leads to all publications available partly in full text via the CERN database.

Theme 1: Group IV Semiconductors

Within the materials investigated, apart from silicon, the most important material in present and future device technologies, considerable attention is given to group IV-IV alloys and diamond. Generally, the role of impurities is investigated, comprising dopants, which control the electrical or optical properties, and harmful but ubiquitously present impurities. In contrast to their lattice location and role under thermodynamic equilibrium conditions, in ion implantations the impurities are often found also to be located in unusual lattice sites and consequently have different properties. A profound understanding of such defects is therefore not only of interest in its own right but of importance also for device technologies, where ion implantation is the preferred doping technique.

1. Radiotracer diffusion studies (IS372, IS380, IS395)

Conventional radiotracer techniques comprise the following steps, which are usually done in different facilities: (i) deposition of the radioisotopes onto the specimen surface, (ii) diffusion annealing, (iii) serial sectioning of the specimens, (iv) sectional recording of the radioactivity for diffusion-profile construction, and (v) extraction of the diffusion coefficients from the diffusion profiles. An improvement is achieved [1] by replacing step (i) with the implantation of the radiotracer into the specimens to a depth (20-100 nm) beyond a potentially modified surface region. To ensure that in step (iv) the radioactivity still lies above its detection limit, the time elapsed since the implantation must not exceed several half-lives. This limits the applicability of conventional techniques to radioisotopes with $T_{1/2} > 1$d. This limitation has recently been removed by developing a novel set-up that allows to measure diffusion coefficients of short-lived isotopes (5 min $\lesssim T_{1/2} \lesssim$ 1 d) on-line at ISOLDE: Instead of step (i), the radioisotopes are implanted into the specimens and steps (ii) and (iii) are done immediately afterwards. The specimens are mounted in a vacuum chamber, flanged to the ISOLDE beam-line, and implantation, diffusion annealing, and serial sectioning by ion-beam sputtering are done in situ.

Using the novel technique, the diffusivities of ^{11}C ($T_{1/2}$ = 20min) and ^{31}Si ($T_{1/2}$ =2.6h) have been successfully measured in semiconductors and amorphous Si-B-C-N ceramics. Future plans will comprise Si-Ge alloys, which are of increasing importance in device technologies, and of which high-quality samples are available now. Here the expected changeover of the self-diffusion mechanism from a predominant interstitialcy mechanism (Si) to a vacancy mechanism (Ge) is to be explored (with ^{71}Ge [2] and ^{31}Si isotopes). It is evident that the applicability of short-lived isotopes of elements only available at ISOLDE in the necessary purity and intensity will enlarge the scope of diffusion studies in general.

2. Lattice location of impurities by emission channeling (EC) (IS310, IS368)

Two groups have been or are actively pursuing such studies, focussing on, respectively, donor and other impurities in diamond and on light or transition metal and rare earth impurities in silicon. In order to understand how impurities affect the electrical and optical properties, as a first step their lattice location has to be known. Often dopant concentrations or the solubility of, e.g., transition metals, in the matrix is by far too low for the application of conventional ion channeling techniques. However, doping (implantation of $\geq 10^{12}$ cm^{-2}) with radioactive isotopes, which emit α-, β^+-, β^-- particles or conversion electrons in their decay, enables to detect channeling/blocking effects of these particles along low-index crystal directions on their path to the surface with much higher sensitivity. The anisotropic emission from the crystal surface depends in a characteristic way on the lattice location of the emitting

atoms, which is thus determined. In a dedicated emission-channeling set-up a position sensitive detector, developed by CERN, is employed for simultaneous measurements over large solid angles; a more advanced detector with higher counting capacity is being developed.

Comprehensive studies of the lattice location, in particular of potential donor impurities in diamond, have been performed, complemented by perturbed γ-γ or γ-e^--angular correlation measurements [3]. In silicon the lattice location of Cu upon implantation at 297 K was found to be near-substitutional sites [4]. Upon annealing at 200^o C different site changes occur in highly doped p- or n-type material, respectively, to random positions and to perfect substitutional sites (cf. the introduction). Similar studies for Fe and Ag impurities are under way.

In likewise detailed studies of Er impurities, which introduce luminescence centres in silicon, these were shown to be located on tetrahedral interstitial sites but could be removed from these sites by pairing with co-doped O atoms, a process known to enhance the luminescence intensity [5]. Future work will concentrate on III-V and II-VI wide-gap semiconductors, where, compared to silicon, very little is presently known about the lattice location of important dopants. The emission channeling technique is rather universal because suitable isotopes with particle emission of sufficient energy are found for the majority of elements of interest. First results have been obtained for ion-implanted Fe in GaN as reported under theme 2.

3. Electron paramagnetic resonance (EPR) studies with radioactive isotopes (P83)

The well-known EPR technique enables a detailed characterisation of the atomic structure and electronic configuration of defects and stable impurities. However, the technique can benefit from the application of radioactive isotopes for an unambiguous identification of defects involving impurities, and also in cases, where probe atoms with different spins, quadrupole moments, or masses are of importance. The group set out for such studies of ^{105}Cd in silicon, decaying to Ag and Pd. The first experiment in 1998 failed due to unexpected out-diffusion of the implanted probe atoms during the necessary annealing procedure. Improved techniques were then tested successfully with stable Cd, In, Ag, and Pd isotopes, and also the EPR sensitivity could be improved [6]. However for man-power reasons and other duties, the group has terminated its activity at ISOLDE.

4. Photoluminescence (PL), deep level transient spectroscopy (DLTS) and EPR studies of Au- and Pt-related defects (IS357)

The project is aimed at the identification and characterisation of Au and Pt impurities in crystalline silicon. It includes studies of homo- or hetero-nuclear pairs as well as their complexes with other common impurities like iron and lithium. The combination of the powerful spectroscopic techniques of photoluminescence (PL), deep level transient spectroscopy (DLTS), and magnetic resonance (EPR) being used to discover new information not obtainable by any other means. The decay of radioactive isotopes through a decay chain provides great finesse in the study of particular defect families and has been particularly rewarding in PL and DLTS because the identification of the nature of a defect is difficult otherwise. Thus many false assignments carrying wide acceptance in the literature have been refuted, and various new results have been obtained [7]. Complexes formed with Pt-Fe, Au-Fe, and Au-Li_2 have been identified by PL and three band gap level of Pt by DLTS, a new

acceptor level assigned to Au and, for the first time, levels related to Ir, Os, and W. In the future, the group wants to extend these studies to further technologically relevant impurities.

5. Mössbauer studies (MS) of Fe in silicon (IS359)

Implantations of ^{57}Mn ($T_{1/2}$ = 1.5 min) at elevated temperatures lead to an annealing of the radiation damage arising from the implantation during the ^{57}Mn lifetime and to their substitutional incorporation in silicon. The decay to the excited 14 keV Mössbauer state of ^{57m}Fe imparts an average recoil energy of 40 eV on the daughter atom, which expels a sizeable fraction into tetrahedral interstitial sites. Thus both isolated substitutional and interstitial Fe can be studied at temperatures unattainable by other techniques [8]. Interstitial Fe has a deep donor level in the band gap and is in the neutral or ionised state depending on the Fermi-level of the material. Thus the electron densities at the nucleus of $Fe_i^{0/+}$ and the lattice vibrational properties have been determined by MS as well as those for substitutional Fe, which was shown not to have a band gap state. These results are in excellent agreement with theoretical predictions. A few diffusional jumps of interstitial Fe during the lifetime of the Mössbauer state (140 ns) cause a line broadening, which is directly proportional to the diffusivity [9]. Thus the controversial issue of a charge state dependence of the $Fe_i^{0/+}$ diffusivity has been resolved; below 600 K the Fe_i^+ diffusivity is larger than that of Fe_i^0 by an order of magnitude (cf. the introduction). At higher temperatures, interstitial Fe (in a near-substitutional site) forms a meta-stable pair with the vacancy, which is created simultaneously in the recoil process. Presumably, this defect has been seen previously by EPR and also in the EC experiments, described above, and is common to Fe and other 3d impurities. Similar, but much less detailed MS results have been obtained in analogous experiments at the RIKEN facility in Japan [10], where a higher beam energy but three orders of magnitude lower intensity is available. The intensity at ISOLDE, > 10^8 ions/s, was fully exploited by the application of a novel resonance detector developed during these experiments. It is evident that the potential is large with this new probe atom for MS to explore further the rich physics of the technologically important Fe impurities in silicon and silicon-based alloys. The studies have been extended to epitaxially grown Si-Ge alloys, SiC, and diamond and will in the future also include studies of gettering processes, i.e. the means to render harmless 3d impurities in devices.

[1] R. Fisher, W. Frank, and K. Lyotovitch, Physica B **273-274**, 598 (1999).
[2] A. Strohm, T. Voss, W. Frank, J. Räisänen, and M. Dietrich, Physica B **308-310**, 542 (2001).
[3] K. Bharuth-Ram, A. Burchard, M. Deicher, K. Freitag, H. Hofsäss, S.G. Jahn, R. Magerle, H. Quintel, M. Restle, C. Ronning, and the ISOLDE Collaboration, Hyp. Int. C **1**, 212 (1996).
[4] U. Wahl, A. Vantomme, G. Langouche, J.P. Araujo, L. Peralta, J.G. Correia, and the ISOLDE Collaboration, Phys. Rev. Lett. **77**, 2142 (2000).
[5] U. Wahl, A. Vantomme, G. Langouche, J.G. Correia and the ISOLDE Collaboration, Journ. Lumisc. **80**, 303 (1999).
[6] W. Näser, W. Gehlhoff, and H. Overhoff, Physica B **273-274**, 279 (1999).
[7] M.O. Henry, M. Deicher, R. Magerle, E. McGlynn, A. Stötzler, Hyp. Int. **120**, 443 (1999).
[8] H.P. Gunnlaugsson, M. Dietrich, M. Fanciulli, K. Bharuth-Ram, R. Sielemann, G. Weyer, and the ISOLDE Collaboration, Nucl. Instr. Meth. B **186**, 55 (2001).

[9] H.P. Gunnlaugsson, M. Dietrich, M. Fanciulli, K. Bharuth-Ram, R. Sielemann, G. Weyer, and the ISOLDE Collaboration, subm. to Appl. Phys. Lett.
[10] Y. Kobayashi, Y. Yoshida, A. Yoshida, Y. Watanabe, K. Hayakawa, K. Yukihira, F. Shimura, and F. Ambe, Hyp. Int. **126**, 417 (2000).

Theme 2: III-V Semiconductors

The III-V semiconductors such as GaAs, InP, GaN and their mixtures are the most important class of semiconductors used in today's high-frequency and optoelectronic devices like microwave devices for communication, LEDs and laser diodes. Especially GaN is the most promising material for optoelectronic applications in the blue and near-UV range.

In contrast to the elemental semiconductors like Si or Ge, impurities can occupy lattice sites both on the group III and the group V sublattice resulting in different electrical and optical properties of the same impurity. Especially after ion implantation the introduced impurities are found to be located at unusual lattice sites. Moreover, even in the pure III-V system not only vacancies or interstitial atoms exist as intrinsic defects but also the so-called antisite defects, a group III atom on a group V lattice site or vice versa, alter the properties of the semiconductor.

In order to build optoelectronic devices it is necessary to dope the materials sufficiently p- and n-type for fabricating p-n junctions. For all wide-band gap compounds, however, doping limitations and compensation phenomena are typical, especially sufficient p-type doping is difficult to achieve. To understand and to optimize the doping by ion implantation, ISOLDE offers many different radioactive isotopes in combination with a large number of different experimental techniques: For the determination of the structure of defects on an atomic scale along with their mutual interaction the $\gamma\gamma$ angular correlation spectroscopy (PAC), for the investigation of diffusion mechanisms the tracer diffusion technique, for the localization of impurity atoms in the lattice the emission channeling technique (EC), for the characterization of the resulting electrical properties Hall effect / resistivity measurements (HE), and for the optical properties photoluminescence spectroscopy (PL). The results reveal that the combination of classic techniques of semiconductor physics on one hand with radioactive ions and nuclear methods on the other hand constitutes a powerful tool for the study of impurities since the specific decay constants of the radioactive isotopes endow the classical techniques with the lacking chemical sensitivity.

Besides from defects created by doping these materials by ion implantation, there is still a lack of knowledge on the intrinsic diffusion behavior of the elements forming the III-V semiconductor like As in GaAs.

A unique impurity influencing all electrically active dopants in III-V semiconductors is hydrogen and its control is crucial in device manufacturing where it is present in many procedures required for material growth, doping, and device structuring.

In the following a brief overview will be given on experiments performed at ISOLDE using radioactive dopants and the type of information you can gain concerning the identification of defects, their lattice location, the interaction between defects, their diffusional behavior, and their optical and electrical properties.

1. Radiotracer diffusion (IS362)

Diffusion in crystals is usually mediated by native point defects; in compounds like GaAs these defects responsible for long range migration can be Ga vacancies, As vacancies, Ga interstitials, and As interstitials. Global aim of the project was to study diffusion processes in technologically important III-V semiconductors such as GaAs and GaN. It was intended to obtain diffusion data with pertinent relevance to semiconductor crystal growth as well as to the fabrication of (opto-) electronic devices. Specifically it was planned to investigate self-diffusion on the As-sublattice of GaAs and its dependence on background doping to gain

information about type and charge state(s) of the As-related point defects involved. Similar data for the Ga sublattice were recently obtained from diffusion experiments on ^{69}GaAs/^{71}GaAs stable-isotope heterostructures by means of secondary ion mass spectroscopy [1,2]. By contrast, there is no other stable arsenic isotope than ^{75}As which constitutes the natural element. Therefore, the only available alternative was the use of a radioactive As tracer for diffusion. Earlier results from the radiotracer method suffered from the short half-life of the employed ^{76}As isotope and its supply from an ambient vapor phase during diffusion. In this context the implantation of the much more suitable long-lived isotope ^{73}As at the ISOLDE facility offered a unique opportunity.

^{73}As diffusion experiments in doped and undoped GaAs [3,4] as well as in epitaxially grown GaN layers were carried out in Münster following the implantation at ISOLDE. Numerical analysis of the observed profile broadening yielded As diffusion coefficients in the temperature range from 900°C to 1000°C (s. Introduction Fig. 1), not only for intrinsic GaAs but also for n-doped and p-doped crystals. A very weak doping dependence was observed, which points to a dominant contribution of an electrically neutral native defect to As diffusion in GaAs. In the case of GaN it turned out that implanted ^{73}As was virtually immobile up to temperatures of about 1300°C. Additional information about As diffusion in GaAs resulted from the broadening of buried nitrogen doping layers in epitaxially grown GaAs/GaAs:N/GaAs heterostructures [5] which was investigated in collaboration with two research groups at the Chalmers University of Technology in Göteborg / Sweden. The relevance of this topic relied on the novel finding that N in GaAs diffuses via the kick-out mechanism in which As interstitials play a major role by mediating the N substitutional-interstitial interchange. The As interstitial component of As tracer diffusion in intrinsic GaAs was deduced from quantitative analyses of the N depth distributions and found to obey an Arrhenius equation with an activation energy of 3.88 eV and a pre-exponential factor of 0.25 cm^2s^{-1} in the temperature range from 700°C to 900°C. It is remarkable that also the above mentioned As tracer diffusion coefficients in intrinsic GaAs are well described by this equation.

Combining the results from ^{73}As and N diffusion leads to the view that diffusion processes on the As sublattice in GaAs are controlled by electrically neutral As interstitials, whereas As vacancies seem to play a minor role at most.

2. Acceptor-Hydrogen interaction (IS312, IS345)

Interstitial impurities such as transition metals and hydrogen atoms most easily influence the properties of semiconductors due to their high mobility. Among the interstitial impurities, playing a role in context with the electronic and optical behavior of semiconductors, hydrogen represents a very important impurity in all semiconductors [6], both from the technical and the scientific point of view. During various manufacturing steps hydrogen is easily unintentionally incorporated in semiconducting material where it efficiently interacts with extrinsic and intrinsic defects. In semiconductors, hydrogen occurs ionized (H^+, H^-), as a neutral atom (H^0), as a stable molecule (H_2), a metastable molecule (H_2*) or as precipitates (H-platelets). During the last years, PAC experiments have been performed to study H in III-V semiconductors using the probe atom ^{111m}Cd acting as acceptor in these materials.. A considerable amount of new information could be provided concerning formation, microscopic structure and stability of acceptor hydrogen complexes [7].

Following the implantation doping and annealing, hydrogen was introduced with help of a low energy (100 eV - 400 eV, doses 10^{14} – 10^{15} cm^{-2})) mass-separated ion beam. This procedure minimizes the production of lattice defects and avoids the introduction of ions other

than hydrogen. The observed characteristic electric field gradients (EFG) shows that under these conditions hydrogen atoms form pairs with up to 80% of all ^{111m}Cd acceptors in GaAs [8], InP, GaP [9], InAs [10], and InSb [11]. These pairs are characterized by an axially symmetric EFG and are oriented along <111> lattice directions. This result is consistent with the generally accepted model proposed by Pajot for III-V semiconductors that the hydrogen atom breaks the Cd-group V bond and saturates the dangling group V bond, whereby the free hole annihilates the Cd dangling bond ('bond center site'). As a consequence, the Cd acceptor and the neighboring group V host atom relax along a <111> direction, whereby the trigonal symmetry is maintained as confirmed by the axial symmetry of the EFG. The stability of the formed Cd-H pairs was determined by analyzing the fraction of pairs measured during an isochronal annealing sequence. As an example, annealing of GaAs at about 450 K leads to the complete dissociation of all Cd-H pairs. This temperature corresponds to a dissociation enthalpy of 1.35(1) eV for the Cd-H pair.

In contrast to cubic systems such as GaAs and InP, GaN possesses a wurtzide structure and therefore gives rise to different configurations of Cd-H pairs [12], parallel and perpendicular to the c-axis of the crystal, which exhibit significantly different stabilities.

3. Hydrogen diffusion (IS345)

A question of fundamental interest in semiconductor physics is the diffusion of hydrogen. Especially in III-V semiconductors, the results obtained by conventional techniques like effusion measurements or SIMS profiling using deuterium are rather puzzling. Even for nominally identically doped materials the published diffusion data are very different. This is most probably due to the fact that hydrogen can exist in different charge states in semiconductors, their population depending on the size of the band gap and the doping, and the interaction between hydrogen and other charged impurities present in the material.

In some specific cases, the diffusion mechanism of hydrogen can be studied on a microscopic scale with PAC spectroscopy [13]. The PAC probe atom ^{117}Cd/^{117}In enables such experiments in III-V compounds. The parent isotope ^{117}Cd represents an acceptor being able to trap hydrogen. After the radioactive decay, the daughter ^{117}In isotopes represent isoelectronic lattice atoms and no binding exists any more between hydrogen and the PAC probe atoms. Due to the characteristic electric field gradient (EFG) created by H present in the neighborhood of ^{117}In (s. Introduction IA Fig. 3), the free hydrogen diffusion could be observed as function of temperature within the time window of about 100 ns defined by the nuclear life-time of the excited state used for the PAC measurement. Both for InP and GaAs a migration enthalpy for the free hydrogen diffusion of about 200 meV could be determined. This measurements have only be possible due to the development of the laser ion source at ISOLDE.

4. Lattice location of impurities (IS342, IS368)

The emission channeling method [14] delivers information about the lattice location of radioactive impurity atoms and via the temperature dependence of the observed site occupations information about the diffusion of these impurities. Due to the detection of charged particles emitted during the radioactive decay, the technique can be performed at much lower impurity concentrations if compared with conventional channeling techniques: Thus, only $10^{10} - 10^{13}$ cm^{-2} radioactive ions are needed, what corresponds to concentrations of $10^{16} - 10^{18}$ cm^{-3} using an implantation energy of 60 keV typical at ISOLDE. This concentration range covers the technically relevant dopant concentrations in semiconductors

and, thereby, warrants a high degree of applicability. By comparing the experimentally determined emission yields with theoretical computer simulations, performed for different lattice sites, the actual lattice sites of the impurity atoms can be determined with high accuracy.

In many semiconductors, Li diffuses very fast and acts as shallow acceptor located on interstitial sites. Due to its low solubility Li is preferentially bound to lattice defects and impurity atoms, which can be used to passivate unwanted electrically active defects. Using the probe atom ^{8}Li, emission channeling measurements determined its lattice site, its diffusional behavior, and its interaction with other defects for many III-V semiconductors. For all studied III-V semiconductors [15], at a certain temperature a transition of Li from interstitial to substitutional lattice sites was observed. This transition temperature allows the determination of the activation enthalpy for the diffusion of the Li impurities. For Li in GaN [16] and AlN this transition happens at 700 K corresponding to an activation enthalpy of 1.7 eV.

Transition metals (TMs) form so-called deep centers in semiconductors, i.e. they introduce levels deep in the band gap of the material, which may trap charge carriers and hence reduce the electrical conductivity. For semiconductor technology, TMs are important in two aspects. On the one hand, they are common contaminants in many manufacturing steps which are easily introduced into the material and diffuse very rapidly. The second important aspect of TMs in semiconductor technology is related to the production of semi-isolating III-V materials. Here the ability of TMs to introduce deep centers is beneficially used to produce material of extremely high resistivity. Emission channeling experiments with ^{59}Fe in GaN [17] gave direct evidence that Fe is incorporated on substitutional Ga sites following ion implantation. These experiments shall be extended to the probe atoms ^{67}Cu and ^{111}Ag implanted into III-V semiconductors.

Rare earth doped semiconductors can be used to produce light emitting diodes where the light output is concentrated in a narrow frequency regime. This behavior is due to the fact that the atomic transitions of rare earth elements are only slightly dependent on their chemical surroundings. In most semiconductors, with the exception of GaN and AlN, characteristic luminescence from rare earths is only observed in the infrared region of the spectrum. Most attention has been focused on the element erbium, which shows luminescence at a wavelength that is a widely used standard in optical telecommunications by means of glass fibers. While Er-doped Si diodes have already been realized, the light output was still too low for technical applications. Considerable interest has recently focused on the luminescence behavior of rare earth impurities in GaN and AlN. It could be shown that by doping GaN with Pr, Er and Tm, light-emitting diodes (LEDs) in the red, green and blue region of the optical spectrum, can be produced. Such devices are especially interesting with respect to the construction of flat panel displays, and, possibly, even lasers. Other rare earth elements which have been experimentally observed to modify the light output from GaN LEDs are Eu, Dy, Sm, Ho and Tb. Using emission channeling, it has been shown that the probe atom ^{143}Pr occupies substitutional Ga sites following room-temperature implantation into GaN and annealing up to 900°C [18]. In the future, it is intended to do high-precision lattice location studies of rare earths in GaN, AlN, and InN. Possible probe atoms in that respect are ^{141}Ce, ^{143}Pr, ^{147}Nd, ^{149}Pm, ^{153}Sm, ^{157}Eu, ^{159}Gd, ^{160}Tb, and ^{169}Yb.

5. Optical and electrical studies of defects (IS345, IS391, P104, P146)

The microscopic insights obtained by nuclear techniques like PAC or EC have to be linked to the optical and electrical properties of the semiconductor under study. This requires the characterization of identically prepared samples by Hall-effect (HE), deep-level transient

spectroscopy (DLTS) and photoluminescence (PL) measurements. Using stable isotopes and identical implantation and annealing conditions, this can be done using any ion implanter. These spectroscopic techniques are able to detect and characterize band gap states but do not reveal direct information about their microscopic origin. To overcome this chemical 'blindness', radioactive isotopes are being used as a 'tracer', i.e. the doping is done with a radioactive isotope instead of a stable isotope of the element of interest. Because of its characteristic concentration change according to the nuclear decay law, the involvement of a radioisotope in an experimentally observed band gap state can be confirmed or denied definitely by several subsequent spectroscopic measurements during the elemental transmutation. Band gap states related to either the parent or the daughter isotope are uniquely identified by their decreasing or increasing concentration, respectively, which is reflected in the change of electrical or optical properties of the sample.

5.1 Doping of GaN and identification of defects

Ion implantation is always accompanied by structural damage to the crystal requiring thermal annealing to achieve electrical activation of the dopants. The reconstruction of the GaN lattice with a melting point of about 2800 K requires annealing temperatures up to 1900 K and an external N_2 overpressure of several GPa to suppress the decomposition of the GaN due to the loss of N. This procedure is not usable for device production, i.e. annealing procedures has to be developed which allow at lower annealing temperatures at least a partially electrical and optical activation of the implanted dopants. Using the acceptors ^{111m}Cd and ^{112}Cd and the double acceptor ^{111}Ag decaying to ^{111}Cd, the reduction of implantation damage, the optical and electrical activation of the implants have been observed using PAC, PL, and HE as a function of annealing temperature using different annealing methods [19,20,21]. The use of N_2 or NH_3 atmosphere during annealing allows temperatures up to 1323 K and 1373 K, respectively, but above 1200 K a strong loss of Cd from the GaN has been observed. Annealing GaN together with elementary Al forms a protective layer on the GaN surface allowing annealing temperatures up to 1570 K resulting in about 10% of the implants acting as dopants [22].

Using the radioactive isotopes ^{71}As, ^{72}Se, ^{77}Br, ^{191}Pt, and ^{197}Hg in combination with PL, it was possible to unambiguously identify the optical transitions in GaN related to these elements and their decay products [23,24].

About ten years after the realization of p-type conductivity of GaN, the p-type doping is still difficult, inefficient and poorly understood. The most commonly used p-type dopant is Mg which substitutes on Ga sites. But almost two orders of magnitude higher atomic concentrations of Mg must be incorporated to get a sufficient hole concentration at room temperature. This means, that 99% of the Mg is compensated or passivated by formation of Mg-defect complexes. Theoretical considerations [25] show that Be may be a more promising candidate for p-type doping. ISOLDE gives the possibility to make use of the radioactive decay of ^{7}Be into Li and ^{28}Mg which decays via a short living Al isotope into stable Si. Using the power of the classical semiconductor spectroscopy techniques in combination with radioactive dopants, it will be possible to discriminate between optical and electrical properties created by the dopants and defects related to the implantation and annealing procedure. The use of radioactive dopants also allows the accurate determination of the fraction of electrically activated p-type dopants for different annealing procedures.

5.2 Antisite defects in GaAs and GaN

An important class of intrinsic defects in a compound semiconductor of type AB like GaAs or GaN are antisites where an A atom is placed on a B site (A_B) or vice versa. Such defects might form during non-stochiometric crystal growth conditions or during particle irradiation or implantation and it is an important topic to know the energy levels of these defects. It is still an open question what the levels of the Ga_{As} antisite in GaAs are and it is even not clear if the Ga_N antisite in GaN exists at all. From valence arguments Ga_{As} or Ga_N should act as a double acceptor.

A unique way to create Ga_{As} or Ga_N antisite defects in a controlled way and to avoid the introduction of any other defect during the production process is the transmutation of radioactive ^{71}As to stable ^{71}Ga.

In a first set of experiments it has been shown [26,27], that none of the PL transitions associated in the literature with Ga_{As} is observed after the transmutation from $^{71}As_{As}$ to $^{71}Ga_{As}$. Therefore, it can exclude that any of these defect lines is caused by an isolated Ga_{As} antisite. Even more puzzling is the fact, that no new PL line appearing between 0.9 eV and 1.515 eV has been observed during the population of the Ga_{As} sites. One possible explanation is that the emission related to Ga_{As} is very weak or very broad and therefore difficult to discriminate against the background due to contamination present in the sample, mainly C and Cu.

Almost nothing is known about the Ga_N antisite in GaN. Different theoretical investigations calculate the Ga_N antisite level at 0.7 eV or at around 1.4 eV above the valence band. It. may also be possible, that antisites in GaN are energetically less favorable than in other III-V semiconductors [28]. In a first experiment using ^{71}As, no PL transitions related to the Ga_N antisite has been found [23] (s. Introduction IA Fig. 7), but this experiment must be repeated and completed by DLTS and Hall effect measurements. A non-existent PL transition does not exclude the existence of the antisite, because the related transitions could be non-radiating.

[1] L. Wang, L. Hsu, E.E. Haller, J.W. Erickson, A. Fischer, K. Eberl, and M. Cardona, Phys. Rev. Lett. **76**, 2342 (1996).
[2] T.Y. Tan, H.M. You, S.Yu, U.M. Gösele, W. Jäger, D.W. Boeringer, F. Zypman, R. Tsu, and S.-T. Lee, J. Appl. Phys. **72**, 5206 (1992).
[3] G. Bösker, N.A. Stolwijk, H. Mehrer, A. Burchard, and U. Södervall, Mat. Res. Soc. Symp. Proc. **528**, 347 (1998).
[4] G. Bösker, J. Pöpping, N.A. Stolwijk, H. Mehrer, U. Södervall, J.V. Thordson, T.G. Andersson, and A. Burchard, Hyperfine Interactions **129**, 337 (2000).
[5] G. Bösker, N.A. Stolwijk, H. Mehrer, J.V. Thordson, U. Södervall, and T.G. Andersson, Phys. Rev. Lett., **81**, 3443 (1998).
[6] S.J. Pearton (ed.): *Hydrogen in Compound Semiconductors*, Mat. Science. For. **148 - 149**, (Trans Tech Publications, Aedermannsdorf, 1994).
[7] M. Deicher and W. Pfeiffer, in ref. [6] p. 481
[8] W. Pfeiffer, M. Deicher, R. Keller, R. Magerle, E. Recknagel, H. Skudlik, Th. Wichert, H. Wolf, D. Forkel, N. Moriya, and R. Kalish, Appl. Phys. Lett. **58**, 1751 (1991).
[9] D. Forkel-Wirth, N. Achtziger, A. Burchard, J.G. Correia, M. Deicher, T. Lich, R. Magerle, J. Meier, W. Pfeiffer, U. Reislöhner, M. Rüb, and W. Witthuhn, in: *Semi-insulating III-V Materials*, M. Godlewski (ed.), (World Scientific, Singapore 1994) p. 267.

[10] D. Forkel-Wirth, A. Burchard, J.C. Correia, M. Deicher, J. Grillenberger, H. Gottschalk, T. Licht, R. Magerle, J. Meier, U. Reislöhner, M. Rüb, and W. Witthuhn, in: *Defects in Semiconductors 18*", M. Suezawa and H. Katayama-Yoshida (ed.), Materials Science Forum (Trans Tech Publications 1995) p. 963.
[11] Doris Forkel-Wirth, N. Achtziger, A. Burchard, J.C. Correia, M. Deicher, T. Licht, R. Magerle, J.G. Marques, J. Meier, W. Pfeiffer, U. Reislöhner, M. Rüb, M. Toulemonde, and W. Witthuhn, Solid State Commun. **93**, 425 (1995).
[12] A. Burchard, M. Deicher, D. Forkel-Wirth, E.E. Haller, R. Magerle, A. Prospero, and R. Stötzler, Materials Research Symposium Proc. **449**, 961 (1997).
[13] A. Burchard, M. Deicher, D. Forkel-Wirth, M. Knopf, R. Magerle, A. Stötzler, V.N. Fedoseyev, and V.I. Mishin, Mat. Res. Soc. Symp. Proc. **513**, 171 (1998).
[14] H. Hofsäss and G. Lindner, Phys. Rep. **210**, 121 (1991).
[15] U. Wahl, Phys. Rep. **280**, 145 (1997).
[16] M. Dalmer, M. Restle, C. Ronning, M. Sebastian, U. Vetter, H. Hofsäss, M.D. Bremser, R.F. Davis, U. Wahl, and K. Bharuth-Ram, J. Appl. Phys. **84**, 3085 (1998).
[17] U. Wahl, A. Vantomme, G. Langouche, J.G. Correia, and L. Peralta, Appl. Phys. Lett. **78**, 3217 (2001).
[18] U. Wahl, A. Vantomme, G. Langouche, J.P. Araújo, L. Peralta, and J.G. Correia, J. Appl. Physi. **88**, 1319 (2000).
[19] C. Ronning, M. Dalmer, M. Deicher, M. Restle, M.D. Bremser, R.F. Davis, and H. Hofsäss, Mat. Res. Sym. Proc. **468**, 407 (1997).
[20] A. Burchard, M. Deicher, D. Forkel-Wirth, E.E. Haller, R. Magerle, A. Prospero, and A. Stötzler, in: *Defects in Semiconductors 19*, G. Davies and M. H. Nazaré (eds.), Materials Science Forum Vol. 258-263 (Trans Tech Publications 1997) p. 1099.
[21] A. Stötzler, R. Weissenborn, and M. Deicher, Physica B **273-274**, 144 (1999).
[22] A. Burchard, E.E. Haller, A. Stötzler, R. Weissenborn, and M. Deicher, Physica B **273-274**, 96 (1999).
[23] A. Stötzler, R. Weissenborn, and M. Deicher, Mat. Res. Symp. Proc. Vol. **595** (2000) W12.9.1 press, and MRS Internet J. Nitride Semicond. Res. **5S1**, W12.9 (2000).
[24] A. Stötzler and M. Deicher, Appl. Phys. Lett., submitted.
[25] F. Bernardini, V. Fiorentini, and A. Boisin, Appl. Phys. Lett. **70**, 2990 (1997).
[26] R. Magerle, A. Burchard, M. Deicher, T. Kerle, W. Pfeiffer, and E. Recknagel, Phys. Rev. Lett. **75**, 1594 (1995).
[27] R. Magerle, A. Burchard, D. Forkel-Wirth, and M. Deicher, in: *Defects in Semiconductors 19*, G. Davies and M. H. Nazaré (eds.), Materials Science Forum Vol. **258-263** (Trans Tech Publications 1997) p. 945.
[28] J. Neugebauer and C.G. Van der Walle, Phys. Rev. B **50**, 8067 (1994).

Theme 3: II-VI Semiconductors

In these materials, in particular in the II-VI semiconductors CdTe, ZnSe, and ZnTe, the influence of intrinsic and extrinsic defects on the electrical and optical properties under implantation conditions will be addressed. In contrast to their behaviour under thermodynamic equilibrium conditions, after ion implantation the introduced impurities are found to be located at unusual lattice sites and consequently exhibit different properties. These investigations are the more important as in II-VI materials the understanding of the interplay between semiconductor properties and defects is much less developed than in the elemental or the III-V compound semiconductors. Besides II-VI semiconductors, ferromagnetic semiconductors of the type AB_2C_4 (with A,C being e.g. group II and VI elements, respectively, and B being Cr) are addressed, which show the coexistence of semiconducting and ferromagnetic properties and are of interest for the field of spinelectronics. For these materials, a brief overview of typical experiments performed at ISOLDE will be given in order to illustrate the type of information that has been obtained.

It should be noted that the success of the investigations presented here has heavily relied on the existence of accompanying experiments at the laboratories in different universities, which actually enabled the efficient use of the limited beam time, offered by the ISOLDE facility.

1. Implantation doping of wide-bandgap II-VI compounds using radioactive dopants

Wide-band gap II-VI compounds are promising for optoelectronics in the visible spectral range for a long time. In order to build the corresponding optoelectronic devices it is necessary to dope the materials sufficiently p and n type for fabricating p-n junctions [1,2]. For wide-band gap II-VI compounds, however, doping limitations and compensation phenomena are typical [3-5]. In particular, conventional doping techniques during growth or by diffusion or implantation reveal stringent doping limits and completely insufficient doping efficiencies [6-10]. In order to address these problems, two projects are active at ISOLDE, which use different radioactive isotopes in combination with a large number of different experimental techniques: For the determination of the structure of defects on an atomic scale along with their mutual interaction the ?-? angular correlation spectroscopy (PAC), for the investigation of diffusion mechanisms the tracer diffusion technique, for the characterization of the resulting electrical properties Hall effect / resistivity measurements (HE) along with capacitance voltage profiling (C-V), and for the optical properties photoluminescence spectroscopy (PL) [11,12].

1.1 Transmutation doping by implantation of host elements (IS325)

From implantation and diffusion experiments on host or isoelectronic elements, annealing conditions were derived in order to remove the implantation damage to a large extent and to achieve a well defined incorporation of the implanted elements. The results show that even the incorporation of implanted host isotopes depends on the native defect state of the II–VI compound samples. This behaviour is caused by various diffusion mechanisms due to the different native defect disorder in chalcogen- and metal-rich materials, respectively. The obtained results further imply that the main reason for inefficiency of conventional doping techniques like ion implantation and diffusion are defect reactions during high-temperature processes, which are avoided here if host elements are incorporated and then transmute into relevant dopants at room temperature. Thus, by performing transmutation experiments, relevant dopants, such as Ag, As, Rb and In, are shown to act as highly efficient acceptors and

donors respectively, if they are incorporated on the correct lattice sites of the metal or chalcogen sublattice and if their immediate environment is free of other defects [13].

Thus, in contrast to conventional Ag doping techniques, for CdTe an uncompensated p-type carrier concentration up to 10^{17} cm^{-3} was reached by transmutation doping. ^{107}Ag dopants were introduced via the radioactive decay of implanted substitutional ^{107}Cd isotopes and act as acceptors with an efficiency of about 100%. The corresponding C-V data confirm this effect: The time dependence of the reverse bias at fixed capacitance increases exactly with the expected half-life of the ^{107}Cd? ^{107}Ag transmutation [14].

1.2 Incorporation and complex formation of dopant atoms (IS369)

From implantation and diffusion experiments on impurity atoms, the technical conditions for the incorporation of electrically active dopants, in particular of acceptor atoms have been investigated. The geometrical and electronic structure of the introduced dopant elements was determined in CdTe, ZnSe, and ZnTe by measuring the electric field gradient (EFG) at suitable radioactive probe atoms using the PAC technique. The radioactive isotopes ^{73}As, ^{77}Br, and ^{111}Ag provided by ISOLDE along with the isotope ^{111}In open the way for PAC investigation of the behaviour of donor and acceptor dopants, respectively, in both sublattices of the II-VI semiconductors. The results obtained with the different probe atoms revealed a consistent microscopic picture of the defect reactions between donor and acceptor defects [15-19]. The information delivered by the experimentally determined EFG was considerably augmented by theoretical calculations of the defect induced EFG using the LAPW method, which delivered information about the electronic charge states of the respective defects along with the accompanying lattice relaxations [20,21] (see also Introduction IA Fig. 5). The access to the latter information is otherwise obtainable only by extended X-ray absorption experiments, but at considerably higher impurity concentrations.

In addition, using PL spectroscopy the properties of the implanted dopants ^{67}Cu, ^{71}As, ^{77}Br, ^{111}Ag, ^{121}Te, ^{132}Cs, and ^{197}Hg were selectively determined by using their respective nuclear lifetime. The experimental results, which again were complemented by theoretical calculations of the respective electronic charge states, supported some of the literature data and, at the same time, contributed to a correction of the interpretation of some of the published PL lines [22,23] (see also Introduction IA Fig. 7). Besides the chemical identification of the different PL signals, the use of radioactive isotopes provided the possibility of varying the defect concentration during the same experiment [24]. In this way, it was possible to determine the radius of excitons and the coupling of acoustic phonons to the excitonic recombination probability.

The investigation of the incorporation of dopants is complemented by tracer diffusion experiments of the dopants ^{111}Ag and ^{67}Cu in CdTe. The measured diffusion profiles show an extremely high mobility of the Ag atoms and, at the same time, a strong repulsive interaction with other defects, being identified as Cu atoms [25]. Thus, Ag atoms implanted at the front side of a crystal are completely pushed to the back side, i.e. across a distance of about 500 µm, by depositing a 20 nm Cu film on the implanted front side and annealing at 550 K for 30 min.

2. Lattice sites and diffusion of impurities observed by emission channelling (IS341)

The emission channelling method delivers information about the lattice location of radioactive impurity atoms and via the temperature dependence of the observed site occupations information about the diffusion of these impurities [26]. Since only 10^{10} – 10^{13}

cm^{-2} radioactive ions are needed, what corresponds to concentrations of $10^{16} – 10^{18}$ cm^{-3} at an ISOLDE typical implantation energy of 60 keV, this technique is able to investigate the technically relevant dopant concentrations in semiconductors and, thereby, warrants a high degree of applicability [12]. By comparing the experimentally determined emission yields with theoretical computer simulations, performed for different lattice sites, the actual lattice sites of the impurity atoms were determined with high accuracy.

In particular, the lattice sites of the atoms Li, Ag, and Cd were studied under various implantation conditions [27-29]. Thus, for the investigation of Ag in CdTe, the radioactive precursors ^{107}Cd and ^{109}Cd were implanted so that after annealing at 600 K the isomeric ^{107m}Ag and ^{109m}Ag can be assumed to occupy substitutional Cd sites. The substitutional fractions of Ag atoms are determined by detecting the emitted conversion electrons which mediate the transition to the ground states of ^{107}Ag and ^{109}Ag [30]. The experimental reveal that around 350 K the Ag atoms start to diffuse, accompanied by a loss of radioactive impurities. These results fit in an excellent way to (i) the high mobility of Ag in CdTe (see 1.2 above) and (ii) the dependence of the incorporation of host atoms (i.e. Cd) on the respective concentrations of intrinsic defects (see 1.1 above), which in this case were controlled via annealing of CdTe in Te or Cd rich environments. - For the investigation of Li in ZnSe, the yield of the emitted a particles due to the decay of ^{8}Li was detected as a function of crystal temperature [31,32]. The channelling data show that the implanted ^{8}Li atoms perform a transition from tetrahedral interstitial to substitutional lattice sites around 300 K. This information fits very well to the corresponding behaviour of ^{8}Li in ZnSe as observed by the ß-NMR technique (see 3. below).

3. NMR study on microscopic structure and diffusion behaviour of Li implanted in ZnSe (P67)

The β-NMR technique is a well established method for providing information on defect properties, such as symmetry, diffusion, and annealing behaviour [33,34]. The use of radioactive isotopes provides an enhancement of the sensitivity, which compared to conventional NMR is many orders of magnitude higher, and is the prerequisite for obtaining information about diamagnetic defects in semiconductors by magnetic resonance. If compared to accelerator based experiments, β-NMR experiments performed at ISOLDE take advantage of much higher count rates and are almost free of background [35,36]. The project, performed at ISOLDE, aims at an improved understanding of the doping problem in II-VI semiconductors and, in particular, studies the role of the acceptor Li in ZnSe by the microscopic investigation of implantation effects [37]. Encouraged by the promising results of these investigations, ISOL-based experiments have meanwhile also been started at TRIUMF (Canada) [38].

Besides N, Li is the only acceptor element giving reproducibly p type conductivity in ZnSe, but with too low a net-acceptor concentration and a limited thermal stability, which both are still not well understood [39]. From emission channelling experiments (see 2. above) the transition of implanted ^{8}Li from an interstitial (I) to a substitutional (S) site is known to occur around 300 K [40]. The ß -NMR data of the ^{8}Li spin relaxation exhibit two minima if measured as a function of temperature. They signal the existence of a third, metastable ^{8}Li configuration, slightly displaced from the S site and invisible to the emission channelling experiments. It is proposed that this third site P represents an inherent, intermediate site between the S an I site that is responsible for the doping problem mentioned above.

4. Doping properties of ferromagnetic semiconductors (IS396)

Magnetic semiconductors should have the best potential for future spin electronic devices what has caused a world wide increase of scientific activities in these materials [41,42]. Since they can easily be coupled to semiconductor layers, the injection of aligned spins into semiconductors should become possible as a first step towards the production and manipulation of spin polarized currents. In the present project the doping properties of different ternary spinel type compounds AB_2C_4 with T_c = 100...430 K are investigated. The large demand for information on a microscopic level can be met by measuring the magnetic and electric fields at the site of the implanted radioactive dopant atoms. For this purpose, experiments with the PAC probes ^{111m}Cd, ^{117}Cd, ^{111}Ag, ^{199m}Hg, and ^{77}Br have been started at ISOLDE [43]. The experiments are complemented by theoretical calculations of the respective magnetic and electric hyperfine fields.

Thus, for the case of $CdCr_2Se_4$, the PAC experiments show that the dopant In after implantation occupies the Cd and the Cr sites [44]. This information is obtained from the EFG and magnetic fields measured above and below T_c, respectively. By using the probe ^{111m}Cd as a reference for the hyperfine fields at the Cd sites, the fields to be expected for ^{111}In at this site are already known, since the hyperfine fields at the site of the implanted ^{111}In atoms are measured after their decay to ^{111}Cd. In general, the present experiments point to the following behaviour: In dopants are substitutes at both cation sites A and B, Cd and Ag occupy the A sites exclusively, and Br atoms are substitutes at the anion sites C.

Developments in the near future

In the technical area, a photoluminescence spectrometer will be built that is capable of studying semiconductors with very different bandgap energies, from Ge up to GaN, SiC, and ZnO, by using an appropriate set of lasers and detectors for excitation and detection, respectively. This system can start its operation as soon as an appropriate lab space is allocated at ISOLDE. This spectrometer together with a ‘semiconductor lab’ at ISOLDE will allow to use short lived radiaoctive isotopes (half-lives down to 1 hour) in semicondcutor physics. Of similar technical importance will be the availability of REX-ISOLDE for implanting radioactive ions at energies up to a few MeV as compared to 60 keV at present.

In the scientific area, new semiconductors materials will be subject of future investigations, such as the II-VI semiconductor ZnO [45] and nano-crystalline semiconductors [46]. Similarly, the field of magnetic semiconductors is just at the beginning of its exploitation. For these materials, first experiments at ISOLDE have already been started.

[1] M.A. Haase, J. Oui, J.M. Depuydt, and H. Cheng, Appl. Phys. Lett. **59**, 1272 (1991).
[2] M. Klude, G. Alexe, C. Kruse, T. Passow, H. Heinke, and D. Hommel, Phys. Stat. Sol. (b) **229**, 935 (2002).
[3] G. Mandel, Phys. Rev. **134 A**, 1073 (1964).
[4] K. Ohkawa, A. Tsujimura, S. Hayashi, S. Yoshii, and T. Mitsuyu, Physica B **185**, 112 (1993).
[5] W. Faschinger, S. Ferreira, H. Sitter, R. Krump, and G. Brunthaler, Mater. Sci. Forum **29**, 182 (1995).
[6] A.N. Georgobiani, M.B. Kotlyarevskii, V.V. Lastovka, and D.A. Noskov, Kratk. Soobshch. Fiz. **6**, 30 (1977).

[7] Y.S. Park, B.K. Shin, D.C. Look, and D.L. Downing, *Proc. 4th Int. Conf. on Ion Implantation in Semiconductors and Other Materials* (Osaka, 1974) ed. S. Namba (New York, Plenum, 1975) p. 245.
[8] S. Adachi and Y. Machi, Japan. J. Appl. Phys. **14**, 1599 (1975).
[9] Y.S. Park and C.H. Chung, Appl. Phys. Lett. **18**, 99 (1971).
[10] S.L. Hou, K. Beck, and J.A. Marley, Appl. Phys. Lett. **14**, 151 (1969).
[11] Th. Wichert, in *Semiconductors and Semimetals* (Academic, New York, 1999), Vol. 51B, Chap. 6.
[12] *Isolde – A Laboratory Portrait*, D. Forkel-Wirth, G. Bollen eds., Hyperfine Interactions **129** (2000).
[13] M. Wienecke, B. Reinhold, J. Röhrich, J. Bollmann, N. Achtziger, U. Reislöhner, W. Witthuhn, S. Hermann, and the ISOLDE Collaboration, J. Phys. D: Appl. Phys. **32**, 291 (1999).
[14] H. Zimmermann, R. Boyn, P. Rudolph, J. Bollmann, A. Klimakow, and R. Krause, Mater. Sci. Eng. B **16**, 139 (1993).
[15] H. Wolf, T. Filz, St. Lauer, A. Jost, V. Ostheimer, Th. Wichert, M. Deicher, R. Magerle, A. Burchard, D. Forkel-Wirth, H.Haas, and the ISOLDE Collaboration, Hyperfine Interactions (C) Proc. **1**, 222 (1995).
[16] H. Wolf, T. Filz, J. Hamann, V. Ostheimer, S. Lany, Th. Wichert, M. Deicher, A. Burchard, and the ISOLDE Collaboration, Mat. Res. Soc. Symp. Proc. **510**, 337 (1998).
[17] H. Wolf, T. Filz, J. Hamann, S. Lany, V. Ostheimer, and Th. Wichert, Physica B **273-274**, 843 (1999).
[18] J. Hamann, A. Burchard, M. Deicher, T. Filz, S. Lany, V. Ostheimer, F. Strasser, H. Wolf, the ISOLDE Collaboration, and Th. Wichert, J. Cryst. Growth **214/215**, 207 (2000).
[19] H. Wolf, T. Filz, V. Ostheimer, J. Hamann, S. Lany, the ISOLDE Collaboration, and Th. Wichert, J. Cryst. Growth **214/215**, 967 (2000).
[20] Stephan Lany, Peter Blaha, Joachim Hamann, Volker Ostheimer, Herbert Wolf, and Thomas Wichert, Phys. Rev. B **62,** R2259 (2000).
[21] S. Lany, V. Ostheimer, H. Wolf, Th. Wichert, and the ISOLDE Collaboration, Physica B **308-310**, 980 (2002).
[22] J. Hamann, A. Burchard, M. Deicher, T. Filz, V. Ostheimer, C. Schmitz, H. Wolf, Th. Wichert, and the ISOLDE Collaboration, Appl. Phys. Lett. **72**, 3029 (1998).
[23] S. Lany, J. Hamann, ISOLDE Collaboration, V. Ostheimer, H. Wolf, and Th. Wichert, Physica B **302/303**, 114 (2001).
[24] J. Hamann, A. Burchard, M. Deicher, T. Filz, V. Ostheimer, F. Strasser, H. Wolf, the ISOLDE Collaboration, and Th. Wichert, Physica B **273-274**, 870 (1999).
[25] H. Wolf, M. Deicher, V. Ostheimer, A. Rodriguez Schachtrup, N.A. Stolwijk, Th. Wichert, and the ISOLDE Collaboration, Physica B **308-310**, 963 (2002).
[26] H. Hofsäss, Hyperfine Interactions **97/98**, 247 (1996).
[27] S.G. Jahn, H. Hofsäss, M. Restle, C. Ronning, H. Quintel, K. Bharuth-Ram, and the ISOLDE Collaboration, in *Ion Beam Modification of Materials*, eds. J.S. Williams, R.G. Elliman, M.C. Ridgway, (Elsevier, Amsterdam, 1996) p. 907.
[28] K. Bharuth-Ram, M. Restle, and H. Hofsäss, Nucl. Instr. Meth B **136**, 751 (1998).
[29] K. Bharuth-Ram, H. Hofsäss, M. Restle, U. Wahl, and the ISOLDE Collaboration, Nucl. Instr. Meth. B **156**, 244 (1999).
[30] S.G. Jahn, H. Hofsäss, M. Restle, C. Ronning, H. Quintel, K. Bharuth-Ram, U. Wahl, and the ISOLDE Collaboration, J. Cryst. Growth **161**, 172 (1996).

[31] M. Restle , M. Dalmer, U. Wahl, H. Hofsäss, and the ISOLDE Collaboration, Mat. Res. Soc. Symp. Proc. **540** (1999).
[32] K. Bharuth-Ram, M. Restle, H. Hofsäss, C. Ronning, U. Wahl, and the ISOLDE Collaboration, Physica B **273**, 875 (1999).
[33] H. Ackermann, P. Heitjans, and H.-J. Stöckmann, in *Hyperfine Interactions of Radioactive Nuclei*, edited by J. Christiansen, Topics in Current Physics Vol. 31 (Springer, Berlin 1983), p. 291.
[34] B. Ittermann, H. Ackermann, E. Diehl, B. Fischer, H.-P. Frank, and H.-J. Stöckmann, Hyp. Int. **79**, 591 (1993).
[35] B. Ittermann, M. Füllgrabe, M. Heemeier, F. Kroll, F. Mai, K. Marbach, P. Meier, D. Peters, G. Welker, W. Geithner, S. Kappertz, S. Wilbert, R. Neugart, P. Lievens, U. Georg, M. Keim, and the ISOLDE Collaboration, Hyperfine Interactions **129**, 423, (2000).
[36] B. Ittermann, M. Füllgrabe, M. Heemeier, F. Kroll, F. Mai, K. Marbach, P. Meier, D. Peters, H. Thiess, G. Welker, H. Ackermann, H.-J. Stöckmann, W.-D. Zeitz, W. Geithner, S. Kappertz, S. Wilbert, R. Neugart, P. Lievens, U. Georg, M. Keim, and the ISOLDE-Collaboration , Hyperfine Interactions **120/121**, 403 (1999).
[37] F. Kroll, B. Ittermann, M. Füllgrabe, F. Mai, K. Marbach, D. Peters, W. Geithner, S. Kappertz, M. Keim, S. Kloos, S. Wilbert, R. Neugart, P. Lievens, U. Georg, and the ISOLDE Collaboration, Physica B, in print (2001).
[38] *TRIUMF Annual Report Scientific Activities 2000*, (Vancouver, 2001).
[39] Y. Marfaing, J. Cryst. Growth **161**, 205 (1996).
[40] K. Bharuth-Ram, M. Restle, H. Hofsäss, C. Ronning, and U. Wahl, Physica B **273-274**, 875 (1999).
[41] K. G. Nikiforov, Prog. Crystal Growth and Charact. **39**, 1 (1999).
[42] H. Ohno, J. Magn. Magn. Mater. **200**, 110 (1999).
[43] V. Samokhvalov, A. Richter, D. Degering, S. Unterricker, M. Dietrich, M. Deicher, I. M., Tiginyanu, Jap. J. Appl. Phys. **39**, Suppl. 39-1**,** 470 (2000).
[44] S. Unterricker, V. Samokhvalov, I. Burlakov, D. Degering, M. Dietrich, M. Deicher, and the ISOLDE Collaboration, Contribution to *12th International Conference on Hyperfine Interaction*, Park City, Utah, August 12 –17, 2001, accepted for Hyperfine Interactions (2002).
[45] C.G. Van de Walle, Phys. Rev. Lett. **85**, 1012 (2000).
[46] Th. Agne, Z. Guan, X.M. Li, H. Wolf, and Th. Wichert, accepted for publication in Phys. Stat. Sol. **B 229** (2002).

Theme 4: Surfaces and Interfaces

1. Introduction

Surfaces and interfaces of solid materials have become a field of tremendously growing interest in several areas of physics, in particular in **ultrathin metallic layer magnetism**. The information on the variation of magnetic properties from atomic layer to atomic layer of ultra-thin multilayer systems or even from atom to atom in such a monolayer is of fundamental interest. Therefore, *local* structural and electronic properties of surfaces and at interfaces measured ***on the atomic scale*** are in the focus of many investigations. The aim is to gain contributions for a better understanding of the overall properties [1].

One way to measure properties on this scale is offered by the use of radioactive probe atoms and the observation of their interaction with the immediate environment measured as hyperfine interactions between the probe nuclei and their electronic structure. The main advantages of **hyperfine interaction measurements**, e.g., performed in perturbed angular correlation spectroscopy **(PAC)** (or Mößbauer spectroscopy)**,** are briefly listed as:

(i) Hyperfine interactions are of short range, therefore monolayer-resolved measurements have been proven to be feasible [2,3].

(ii) The penetration of radiation is of long range, therefore measurements in any depth of a layer system are possible as shown for the Ni/Pd system [4].

(iii) Measurements with nuclear methods are of high sensitivity, only 10^{-5} - 10^{-4} of a monolayer (ML) of radioactive probes are necessary for a measurement, therefore the macroscopic properties of the ML, especially of the layer system, are not influenced by the probes.

2. Opportunities at ISOLDE

ISOLDE delivers a large variety of nuclear probes, as an *on-line* separator it offers especially short-lived probes with half lifes of minutes or hours, therefore a "problem-oriented" choice of probes for solid state experiments is possible [so far, ^{117}Cd, ^{111m}Cd, ^{107}Cd, ^{111}Ag, ^{111}In, ^{77}Br, ^{79}Br, ^{149}Gd as precursors were used in our UHV camber **ASPIC (Apparatus for Surface Physics and Interfaces at CERN)**]. Furthermore, as a *separator* it delivers an extremely clean beam of probe ions, which is necessary for surface and interface experiments and puts the experiments at ISOLDE in a very advantageous position in comparison to laboratory experiments, where chemical separation is nececssary.

3. Competing methods

Competing methods on an atomic scale are given with the development of scanning tunnelling micoscopy, however, this method is restricted essentially to surface investigations.

At large scale facilities, neutron reflectometry is a powerful method to measure magnetic moments directly, but monolayer-resolved measurements are extremely difficult and this method does not distinguish between elements. Element-specific measurements are possible with the determination of magnetic dichroism in photoemission experiments at synchrotrons, although the derivation of magnetic moments is model dependent. All these methods measure the spin (and orbital) polarization of *d* and *p* electrons in magnetic materials, they have little or non access to the *s* electron polarization. Magnetic hyperfine fields, however, are a measure for the *s* electron polarization, since the Fermi contact term of the *s* electrons plays the

dominant role in generating these fields at the (nonmagnetic) probe nuclei. In a theoretical study the interplay between the polarization of *d*, *p*, and *s* electrons was recently demonstrated [see below at 4.1]. In conclusion, hyperfine interaction experiments offer access to local properties and in addition serve as complementary studies for magnetic materials. They present their most valuable contributions in ultrathin systems, where atomic resolution is required. Furthermore, magnetic dipole and electric quadrupole interactions are measured simultaneously, i.e., the identification of the sites of the nuclear probes can be determined simultaneously.

In laboratory experiments, nuclear methods suffer from the lack of a *variety* of suitable probes. In general, only a few can be used, e.g., ^{111}Cd in PAC or ^{57}Fe in Mößbauer spectroscopy (MS).

4. Results at ISOLDE (IS318)

In our experiment IS318 "**Surface and interface studies with radioactive ions**" (completed) we studied semiconductor and magnetic surfaces and magnetic interfaces whereas in IS375 "**Interface magnetism investigated with radioactive atoms**" (in progress) we concentrated on magnetic systems. Out of the large variety of such systems magnetic properties of ultrathin metallic multilayers in Ni/Pd systems were investigated.

Three pioneering experiments using ASPIC at ISOLDE were concentrated on Ni/Pd thin-layer systems, where induced magnetic interactions in Pd were investigated. They are described as follows:

4.1 Surface magnetism studied at adatoms

In a first experiment the surfaces of ferromagnetic Ni and nonmagnetic Pd were compared using isolated radioactive Se adatoms as probes. As result we experimentally found a completely different behaviour for the magnetic hyperfine fields of this probe at surfaces as compared to bulk measurements [5]. This finding prompted a theoretical study mentioned above [6] with a comprehensive explanation including surprising predictions for other elements of the 4*sp* series. In further experiments we could confirm some of these predictions [PhD thesis A. Weber] and observe magnetic hyperfine fields in dependence of the coordination number of the ferromagnetic substrate.

4.2 Induced fluctuating magnetic interactions in Pd

Ni was grown on a Pd single crystal by molecular beam epitaxy (MBE) after PAC probes were positioned in a well defined distance from the Ni/Pd interface. Magnetic interactions of long range could be observed exactly at the position of the probes. This was due to the fact that hyperfine interactions are of short range. The magnetic interactions revealed themselves to be of fluctuating character [4].

4.3 Induced static magnetic interactions in Pd

Pd was grown monolayer by monolayer by MBE on single crystals of Ni with Cd and Pd PAC probes positioned within the terraces of Pd [2]. The *3d-4d* electron hybridization between Ni and Pd differs from Pd atom to Pd atom because of the different lattice parameters for Ni and Pd. For Pd probe atoms we obtained a large distribution in magnetic hyperfine fields, whereas for the Cd impurity PAC probe we obtained discrete fields, surprisingly. Obviously, Cd impurities occupy selected sites within the Pd unit cells. The magnetic

interactions were found to be of static character indicating a ferromagnetic order in Pd. Further experiments are summarized in the PhD thesis of K. Potzger.

5. Future experiments

Future experiments at ASPIC/ISOLDE will be performed at combinations of *3d* and *4f* element systems: In particular we are planning to grow ultrathin layers of Gd on Fe single crystals and perform investigations with magnetic and nonmagnetic radioactive probes, probing the magnetic properties in the immediate neighbourhood of the interface. These experiments shall be performed in cooperation with a research group applying dichroism measurements at the same systems. The perpendicular (?) orientation of moments in Gd with respect to the in-plane orientation in Fe favours possible applications.

[1] Robert C. O'Handley, Modern magnetic materials, John Whily & Sons, New York, 2000, pp 432.
[2] H.H. Bertschat, H.-H. Blaschek, H. Granzer, K. Potzger, S. Seeger, W.-D. Zeitz, H. Niehus, A. Burchard, D. Forkel-Wirth, and ISOLDE – Collaboration, Phys. Rev. Lett. **80**, 2721 (1998).
[3] J. Voigt, X.L. Ding, R. Fink, G. Krausch, B. Luckscheiter, R. Platzer, U. Wöhrmann, and G. Schatz, Phys. Rev. Lett. **66,** 3199 (1991).
[4] H.H. Bertschat, H. Granzer, H. Haas, R. Kowallik, S. Seeger, W.-D. Zeitz, and the ISOLDE - Coll., Phys. Rev. Lett. **78**, 342 (1997).
[5] H. Granzer, H.H. Bertschat, H. Haas and W.-D. Zeitz, J. Lohmüller, G. Schatz, and the ISOLDE - Coll., Phys. Rev. Lett. **77**, 4261 (1996).
[6] Ph. Mavropoulos, N. Stefanou, B. Nonas, R. Zeller, and P. H. Dederichs, Phys. Rev. Lett. **81**, 1505 (1998).

Theme 5: Superconductors, Manganites and Optoelectronic Oxide Materials

Oxide materials show at present great interest in fundamental and applied research due to their large variety of structural, electric and magnetic phenomena. Examples of such are perovskites where high-temperature superconductivity occurs on *cuprates* and giant/colossal magnetoresistance on *manganites*. On the other hand, oxide-insulating ferroelectric materials like $K_{1-x}Li_xTa_{1-y}Nb_yO_3$ (KLTN) and $Pb_xZr_{1-x}TiO_3$, represent two new research materials with interest for optoelectronic devices.

The combination of radioactive nuclear techniques, using radioactive ions only available at ISOLDE, is a very powerful tool to study local phenomena like impurity lattice site and the electronic environment of doping elements. These techniques are particularly relevant when dopants are in low concentrations or are lighter than the crystalline matrixes.

A first proposal was approved at ISOLDE in 1997 for studies on high-Tc superconductors. This was a collaboration of various institutions (ITN/Sacavém, CFNUL/Lisboa, FPG/Leipzig, IKS/Leuven) with well-established traditions on ion beam analysis, ion implantation and studies done at ISOLDE with the complementary e-γ, γ–γ perturbed angular correlation (PAC) and emission channeling (EC) techniques. More recently, other institutions (PDUA/Aveiro, IFIMUP/Porto) with particular expertise of manufacturing and characterizing manganites, have become responsible for a new proposal on this subject at ISOLDE.

Due to the particular material specificity and production difficulties the proposals strongly rely on the collaboration with 10 international institutes, which produce and characterize all samples.

Studies of High-TC Superconductors Doped with Radioactive Isotopes (IS360 since 1997)

Three main topics were proposed:

1) Study of the local environment of ^{199}Hg in $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$, the family of high temperature semiconductor with the highest Tc. The aim is to characterize the local oxygen (O_δ^{2-}) and fluorine (F^-) atoms, which go to the Hg-planes and dope the superconducting CuO_2 planes. So far, quantitative techniques have shown that the doping concentration of O_δ^{2-} (F^-) is about 1.5 bigger than expected for the induced double (single) hole charge carriers. Furthermore, structural anomalies that are possibly related with the superconducting transition, have previously been observed (but not resolved) by neutron diffraction and EXAFS. Using the PAC technique, the vicinity of the apical chain O-Hg-O can be, as well, probed as a function of temperature looking for local structural or charge perturbations.

The experiments successfully provided the local identification of single O_δ atoms that sit in the center of the Hg planes. In addition it was shown the existence of other, not yet identified oxygen-related defects near the Hg planes [1]. These results prove the existence of different oxygen defects near the Hg planes, which could not be resolved by traditional quantitative methods. This work triggered first-principle band structure calculations of the charge distribution in undoped and oxygen doped Hg1201 lattice structures, which well reproduced the experimental data [1]. The calculations have further shown that the electric field gradient (EFG) at the Ba site is extremely sensitive to O_δ. According to cluster calculations of structural doping effects, Ba was predicted to be the vehicle of the charge transfer, even slightly changing site. Therefore, the measurement of the EFGs at the Ba site

can provide in the future relevant information of the charge transfer mechanism. Additional experiments are being prepared to study the F^- doping.

On Hg1201 samples, which were doped with carbon, PAC measured different highly stable EFGs. Actually it is accepted that C doping implies the replacement of the apical dumbbell O-Hg-O^{2-} by CO_3^{2-} ions on two different configurations. The preliminary analysis of our data favors the configuration with one C atom at the Hg place, two oxygen near the apical positions and the third one near the center of the Hg square.

Studies of the temperature dependence of the EFG at the Hg site have been done from 12K to room temperature. It was found that the EFG asymmetry parameter (η) becomes non-zero already below 160K. This is an anomalous behavior for a tetragonal structure, revealing that the charge distribution near the strong linear dumbbell O-Hg-O becomes non-axially symmetric at low temperatures [2]. New results, still unpublished, have shown clear low temperature $\eta \neq 0$ [3]. Experiments are going on to further investigate the origin of the electronic or structural phenomena that influence, in particular, the Hg neighborhood.

2) Study of Hg lattice site stability and diffusion on $YBa_2Cu_3O_{6+x}$ (YBCO). HgO is currently used as an oxygen carrier to optimize Tc in YBCO, being accepted that Hg^{2+} replaces Ba^{2+}, leaving Ba vacancies when Hg diffuses out at high temperature. We have shown, using e^--γ PAC and EC techniques, that Hg is highly stable on YBCO, occupying the Cu(1) site, forming O-Hg-O^{2-} [4,5,6].

3) Study of the ion implantation of Na, K, Rb and Cs into the Infinite Layer Cuprates (ILC) Ca(CuO_2) and Sr(CuO_2). These are the simplest structures of the HTSc, being made of CuO_2 planes alternating with earth-alkaline elements, without charge carrier reservoir. Alkalines cannot be introduced into these materials during growth and, if at the earth-alkaline site, they can be the source of p-type superconductivity. Only during 2001 we got high quality samples (thin films produced by Molecular beam epitaxy at ESCI-Paris) to start experiments in 2002.

Studies of Colossal Magnetoresistive Oxides with Radioactive Isotopes (IS390 since 2001)

Colossal magnetoresistance (CMR) effects on manganese oxides are due to the strong link of the magnetic coupling of manganese ions spins with the lattice and charge dynamics. In general it is assumed that the doping effects and dopant site are associated with the valence and size of the dopant ion. In particular it was assumed that Cd and Ca doping lead to the same effects. Recently it was shown that this is not true. In fact Cd doping leads to a ferromagnetic insulator, while Ca doping leads to a ferromagnetic metal. First results using the EC technique at ISOLDE have shown that Cd atoms on regular lattice sites mainly occupy the Mn site and not the La site. This could not be observed by other techniques like RBS that cannot properly separate the Cd from the La signal. PAC results performed with ^{111}Cd did detect the ferromagnetic transition with great accuracy. In particular, it was shown that at 10K a very strong hyperfine field interacts with Cd. Such studies will continue on $La_{1-x}Cd_xMnO_3$ and $La_{1-x}Ca_xMnO_3$ materials as a function of the Cd and Ca concentration [7].

Study of the lattice site location of copper in $K_{1-x}Li_xTa_{1-y}Nb_yO_3$:Cu (since 2001)

$K_{1-x}Li_xTa_{1-y}Nb_yO_3$ (KTLN) is a compound of current interest due to the possibility of recording holograms by a photo-refractive process, due to the formation of dipolar cluster structures. The rate of creation and stability of the clusters are very sensitive to both the applied field, temperature and doping. In the particular case of Cu and V doped KTLN the

efficiency of the crystalline diffraction depends quadratically on the external applied electric field. This is one more case where traditional techniques cannot identify the lattice site location of Cu.

In 2001, a contract with an industrial partner (*Trellis-Photonics, Israel)*, ITN, IKS and CERN/ISOLDE was signed, aiming to determine the Cu lattice sites, as a function of Cu concentration, on KLTN. For this purpose EC experiments with the ^{67}Cu isotope produced at ISOLDE will be performed. In case the experiments are successful a full proposal should be presented to the INTC. The establishment of a formal contract reflects the need of keeping the intellectual property of the results obtained at ISOLDE, as well as the confidentiality about details on the sample preparation and composition [7].

Piezoelectric materials as $BaTiO_3$ are particularly attractive for optical and holographic storage and optical waveguides. Motivated by previous work [8], by taking advantage of the new PAC isotope, ^{204m}Pb, test experiments on single crystalline thin film material of $Pb_{0.4}Zr_{0.6}TiO_3$, with even higher piezoelectric constants, just have started at ISOLDE (FP, Konstanz) , with the aim of resolving the lattice sites and the amount of Pb^{2+} and Pb^{4+} that determine the material properties.

[1] J.G. Correia *et al.*, Phys. Rev. **B61**, 11 769 (2000).
[2] J.P. Araújo et al., Physica C **341-348**, 1969 (2000).
[3] http://tilde-joao.home.cern.ch/~joao/IS360_add1.pdf.
[4] J.P. Araújo *et al.*, Nucl. Instr. Meth. B **147**, 244 (1998).
[5] J.P. Araújo *et al.*, Nucl. Instr. Meth. B **148**, 807 (1999).
[6] J.P. Araújo *et al.*, in preparation to Phys. Rev. B
[7] see the short scientific report to the annual Project CERN_P_FIS_40125_2000 (FCT/Portugal), http://tilde-joao.home.cern.ch/~joao/CERN_P_FIS_40125_2000_scientific_report_colour.pdf
[8] M. Dietrich, C. Camard, M. Deicher, F. Richter, V. Samokhvalov, S. Unterricker, Z. Naturf. **57a** (2002), in press.

Theme 6: Metals

The observation of hyperfine interactions is well suited to study the electronic state in the local environment of dilute impurity atoms in solids. Using radioactive probe atoms and resonance techniques like Mössbauereffect or nuclear magnetic resonance on oriented nuclei (NMR-ON) the hyperfine parameters (hyperfine fields, electric field gradients, isomer shift and nuclear spin-lattice relaxation) can be determined precisely and site-specific, i.e. separately for substitutional, vacancy associated or interstitional sites. For a successful interpretation of the data excellent samples with very low concentration of the impurity atoms are needed. In addition access to a large variety of isotopes in many cases very short-lived is essential. In some cases more than one isotope of one element with different nuclear moments have to be implanted in one sample. All these requirements are met uniquely by the ISOLDE facility. This will be demonstrated with three examples of recent experiments at ISOLDE:

(i) Spin orbit induced electric field gradients of 5d impurities in ferromagnets
(ii) Electric quadrupole contribution to the nuclear spin-lattice relaxation of Ir in Fe
(iii) Structure and kinetics of vacancies and self-interstitials in ferromagnetic Fe

Spin-orbit induced electric field gradients of 5d impurities in ferromagnets (IS314)

The existence of an electric field gradient (EFG) at the nuclear site of dilute impurity atoms in a cubic host lattice is attributed to an unquenched orbital momentum produced by the spin-orbit interaction of the d electrons of the impurity atom. In order to explore the anisotropy of the spin-orbit EFG the electric quadrupole interaction of ^{188}Ir in an Fe single crystal was measured for magnetization parallel to the crystallographic [100], [110] and [111] axes. Contrary to all previous experiments, a strong dependence of the EFG on the direction of the magnetization with respect to the crystallographic axes was observed for the first time. The sample of ^{188}Ir in Fe was prepared at ISOLDE by implantation of ^{188}Hg with E = 60 keV into an Fe single crystal with high surface quality. The impurity concentration in a layer of ~ 5nm width was ~ 0.05 at%, i.e. the criteria for a dilute alloy are well fulfilled. The quadrupole interaction for different directions of the external field was measured with the technique of modulated adiabatic fast passage on oriented nuclei (MAPON). With this technique it is possible to determine the distribution of the quadrupole splitting even if the inhomogeneous broadening of the magnetic interaction is much larger than the quadrupole splitting. With this unique feature of MAPON to detect very small quadrupole splittings combined with the exceptional possibilities at ISOLDE it was possible to determine the EFG and its anisotropy for a large number of 5d impurities implanted in Fe and Ni. Within the scope of these measurements a quite unexpected behaviour has been found for the system ^{191}Pt in Fe. For magnetization parallel to [111] and [110] the distribution of the EFG is relatively sharp with a unique negative sign, whereas for [100] the EFG is broadly distributed around an average value near zero. For M parallel to [100] the EFG distribution is by a factor of 2.8(6) broader than for M parallel to [111]. Additional data on Os, Re, Ir, and Au in Fe indicate that this behaviour is of general nature: In all cases the EFG distribution for M || [100] is considerably broader than for M || [110] and [111]. The origin of this effect is still unknown. It cannot be due to [100]-lattice defects, since impurity nuclei with a defect in the near neighbourhood do not contribute to the MAPON signal because of their different magnetic interaction. It could be connected with details of the band structure, or - based on the experimental fact, that the broadening is in all cases largest for M || [100] - one could speculate, that it is caused by small charge and/or spin density waves along the [100], [010] and [001] directions. Further experiments are necessary to clarify this situation.

A spin-orbit induced EFG collinear to the magnetization should also be present for hexagonal Co as host in addition to the much larger lattice field gradient. The isotropic part of this spin-orbit induced EFG can be measured for impurities implanted into a hcp-Co single crystal. For the system Ir in hcp-Co a large collinear EFG with negative sign was found. Within the series of the 5d elements Ir, Pt, Au and Hg this is exceptional: The experimental values for Pt, Au and Hg are at least 2 orders of magnitude smaller and consistent with zero.

Electric quadrupole contribution to the nuclear spin lattice relaxation of Ir in Fe (IS314)

The nuclear spin-lattice relaxation (NSLR), the dynamic part of the hyperfine interaction, arises predominantly from the magnetic hyperfine interaction and depends on the density of states at the Fermi energy and on the nuclear magnetic moment μ. A contribution of quadrupole interaction to NSLR, acting on the quadrupole moment Q, was proposed by Obata but was considered to be very small and was neglected in the ab initio calculations of Akai for nd-impurities in Fe as well as in the interpretation of experimental data. On the other hand the theoretical calculation strongly underestimates the experimental relaxation rates (for 5d impurities by a factor of 3, see e.g. [1]). In order to clearup the influence of quadrupole interaction on NSLR an experiment was performed on a sample, which contained two isotopes namely ^{186}Ir and ^{189}Ir. For this purpose ^{186}Hg and ^{189}Hg, the Hg precursors of the Ir isotopes were implanted at ISOLDE into the central part of a disc-shaped Fe single crystal. Due to the strongly different ratios of nuclear moments Q/μ for the two isotopes it was possible to determine the quadrupolar part of the NSLR for the first time. Furthermore it was possible to decompose the magnetic relaxation rate into an orbital and nonorbital part using the fact that the radial part of the matrix elements for the orbital magnetic relaxation and for the quadrupolar relaxation is the same. This orbital part of the relaxation is found to be moderately well described by the theory of Akai [2]. However, contrary to the predictions of the theory, this orbital part is only a minor contribution to the total nuclear spin-lattice relaxation of the 5d impurities in Fe. This is the first direct experimental evidence for the nonorbital nature of the unexpectedly large relaxation rates.

Structure and kinetics of vacancies and self-interstitials in ferromagnets (P97)

The test experiment P97 has had two beam times for testing developed detectors and implantation chambers, and taking the first data. These are of excellent statistical quality but suffer from a complicated line shape of the resonance detector with a stainless steel absorber (enriched in ^{57}Fe), which hampers the quantitative analysis of the spectra. For implantations of ^{57}Mn at 300 K into α-iron a resonance detector with four α-^{57}Fe layers could be applied, resulting in well-controlled line shape. The central line (complete matching of the magnetically-split sextets of emitter and absorber) shows no satellites, thus >99% of the ^{57m}Fe daughter atoms are located on substitutional lattice sites. Spectra from implantations at 77 K do show spectral components (~10%) with magnetic hyperfine fields B_{hf} larger (36 T) and smaller (30-26 T) than for substitutional ^{57m}Fe (33.8 T) and in addition quadrupole interactions and different isomer shifts. Based on alloy data and previous implantation results, the component(s) with a lower B_{hf} are tentatively assigned to vacancy-associated probe atoms, whereas a component (~7%) with a larger B_{hf}, firmly observed here, has never been reported previously – to our knowledge. As these experiments are distinguished from all previous approaches by the 40 eV average decay recoil energy imparted on the ^{57m}Fe daughter atoms, it is tempting to interpret this component as due to interstitial Fe atoms, expelled from substitutional sites by the recoil effect. Given these assignments, the absence of this component at 300 K implies then that recombination takes place within the 140 ns lifetime of

^{57m}Fe. This is consistent with an activation energy (0.3 eV) controlled recombination observed at 110 K on a 10 min time scale (stage IE). This result is consistent with both the “one-interstitial” (1IM) and the “two-interstitial” (2IM) models (cf. [3] for an elaborate review), however, the further interpretation appears in conflict with the 2IM proposed there. At 300 K also no vacancy-related component is observed anymore. Mn impurities are known to bind vacancies at T < 200 K, which become mobile at that temperature within the ^{57}Mn lifetime (2.3 min), according to the 1IM with an activation energy of 0.56 eV. Thus, if created in the implantation process, vacancies can escape from the probe atoms at >200 K. If they are created by the recoil effect, i.e. in a replacement collision with a nearest neighbour atom, as frequently observed in fcc and bcc lattices, they cannot escape within 140 ns and would have to be annihilated by recombination. These processes can be distinguished by their temperature dependencies and data at intermediate temperatures are obviously needed to clarify these issues further. Unfortunately, the breakdown of ISOLDE’s GPS prevented measurements in 2001.

[1] T. Funk et. al., J. Magn. Magn. Mater. 195, 406 (1999).
[2] H. Akai, Hyperfine Interact. 43, 255 (1988).
[3] H.J. Blythe et. al. Phys. Stat. Sol. **(a) 181**, 233 (2000).

III Scientific Output

Publications in refereed journals (last five years)

Diffusion of Gold and Platinum in Amorphous Silicon and Germanium. IS380
W. Frank, W. Gustin, and M. Horz, J. Non-Cryst. Solids 205-207, 208-211 (1996)

Diffusion of Transition Metals in Amorphous Silicon and Germanium. IS380
M. Horz, W. Gustin, P. Scharwaechter, W. Frank, and ISOLDE COLLABORATION, Def. and Diff. Forum 143-147, 729-734 (1997)

Diffusion in Amorphous Solids - Metallic Alloys and Elemental Semiconductors. IS372
W. Frank, Def. and Diff. Forum 143-147, 695-710 (1997)

First Low-Temperature Studies of Diffusion in Icosahedral Quasicrystals. IS372
R. Blüher, P. Scharwaechter, W. Frank, and H. Kronmüller, Phys. Rev. Lett. 80, 1014-1017 (1998)

Diffusion in nichtkristallinen Festkörpern. IS380
W. Frank, P. Scharwaechter, R. Blüher, W. Gustin, M. Horz, S. Matics, and T. Schuler, in: Jahrbuch der Max-Planck-Gesellschaft 1998, edited by the Max-Planck-Gesellschaft, Vandenhoeck und Ruprecht, Göttingen 1998, p. 554-562

Diffusion in Non-Crystalline Solids, Particularly in Metallic Glasses and Quasicrystals. IS372
W. Frank, P. Scharwaechter, and R. Blüher, Proc. 9th Intern. Symp. Continuum Models and Discrete Systems, Istanbul, Turkey, 1998, edited by E. Inan and K.Z. Markov, World Scientific, Singapore 1998, p. 562-569

Diffusion of Gold in Relaxed Si-Ge Epi-Layers. IS380
R. Fischer, W. F. J. Frank, and K. Lyutovich, Physica B 273-274, 598-602 (1999)

Diffusion of ^{103}Pd and ^{195}Au in Icosahedral $Al_{70.2}$ $Pd_{21.3}$ $Mn_{8.5}$ Under Proton Irradiation. IS372
R. Blüher, W. Frank, and B. Grushko: Materials Science and Engineering A 294-296, 689-692 (2000)

Diffusion in Icosahedral Al-Pd-Mn. IS372
W. Frank, R. Blüher, and I. Schmich, Advances in Science and Technology 29 (Mass and Charge Transport in Inorganic Materials - Fundamentals to Devices, edited by P. Vincenzini and V. Buscaglia, Techna, Faenza 2000), 205-212 (2000)

Diffusion of Gold in the Amorphous Ceramic Si_{28} C_{36} N_{36}. IS372
S. Matics and W. Frank, Defect and Diffusion Forum 194-199, 947-952 (2001)

Diffusion of Implanted Radiotracer Atoms ^{195}Au in Amorphous Silicon Under Irradiation with 1 MeV - N^+ Ions. IS380
T. Voss, P. Scharwaechter, W. Frank, and ISOLDE Collaboration, Defect and Diffusion Forum 194-199, 659-666 (2001)

Diffusion of Gold in Germanium. IS380
A. Strohm, S. Matics, and W. Frank, Defect and Diffusion Forum 194-199, 629-634 (2001)

C. Ronning and H. Hofsäss, Diam. Relat. Mater. 8 (1999) 1623-1630 IS310

S.Virdis, U.Vetter, C. Ronning, H. Kröger and H. Hofsäss IS342
J. Appl. Phys. (2002) to be published

Implantation sites of Ce and Gd in diamond. IS342
K. Bharuth-Ram, U. Vetter, H. Hofsäss, C. Ronning and M. Dietrich, 15th Int. Conf. on Ion Beam Analysis, Cairns, Australia. 15-20 July, 2001, Nucl. Instr. Meth. B (2002) to be published

Implantation sites of In, Cd, and Hf in diamond. IS342
K. Bharuth-Ram, A. Burchard, M. Deicher, H. Quintel, M. Restle, H. Hofsäss, and C. Ronning, Phys. Rev. B 64 (2001) 195207

Substitutional Phosphorous Doping of Diamond by Ion Implantation. IS310
H. Hofsäss, M. Dalmer, M. Restle and C. Ronning, J. Appl. Phys. 81 (1997) 2566

Behavior of the Potential n-Type Dopants P and As in Diamond After Low Dose Ion Implantation. IS310
H. Hofsäss, M. Dalmer, M. Restle, C. Ronning, K. Bharuth-Ram, H. Quintel and The ISOLDE-Collaboration, Mat. Res. Soc. Symp. Proc. Vol. 442 (1997) 675-680

Microscopic Studies of Implanted ^{73}As in Diamond: γ-e^- PAC and Emission Channeling Measurements. P66
J.G. Correia, J.G. Marques, E. Alves, D. Forkel-Wirth, S.G. Jahn, M. Restle, M. Dalmer, H. Hofsäss, K. Bharuth-Ram and ISOLDE Collaboration, Nucl. Instr. Meth. B 127/128 (1997) 723

Cathodoluminescence Studies of Ion Implanted Diamond. IS310
H. Sternschulte, T. Albrecht, K. Thonke, R. Sauer, M. Dalmer, C. Ronning and H. Hofsäss, Appl. Phys. Lett. 71 (1997) 2668

Lattice Sites of Li in Si and Ge. IS310
U. Wahl, S.G. Jahn, M. Restle, H. Quintel and H. Hofsäss,
Mat. Sci. For. 196-201, Part 1 (1995) 115-120

Ion implantation Doping of Diamond Studied by PAC. IS310
K. Bharuth-Ram, A. Burchard, M. Deicher, K. Freitag, H. Hofsäss, S.G. Jahn, R. Magerle, H. Quintel, M. Restle, C. Ronning and the ISOLDE Collaboration, Hyperfine Interactions (C) 1 (1996) 212

Emission Channeling Study of Annealing of Radiation Damage in Heavy-ion Implanted Diamond. IS310
H. Quintel, K. Bharuth-Ram, H. Hofsäss, M. Restle, C. Ronning,
Nucl. Instr. Meth. B 118 (1996) 72-75

Emission channeling studies of Li in semiconductors. IS310
U. Wahl and the ISOLDE collaboration
Physics Reports 280 (1997) 145-285.

Direct evidence for tetrahedral interstitial Er in Si. IS368
U. Wahl, A. Vantomme, J. De Wachter, R. Moons, G. Langouche, J.G. Marques, J.G. Correia and the ISOLDE collaboration
Physical Review Letters 79 (1997) 2069-2072.

Lattice sites and damage annealing of implanted Tm and Er in Si. IS368
U. Wahl, J.G. Correia, J. De Wachter, G. Langouche, J.G. Marques, R. Moons, A. Vantomme, and the ISOLDE collaboration
Materials Research Society Proceedings 469 (1997) 407-412.

Direct evidence for stability of tetrahedral interstitial Er in Si up to 900°C. IS368
U. Wahl, J.G. Correia, G. Langouche, J.G. Marques, A. Vantomme and the ISOLDE collaboration
Materials Science Forum 258-263 (1997) 1503-1508.

Electron emission channeling with position-sensitive detectors. IS368
U. Wahl, J.G. Correia, S. Cardoso, J.G. Marques, A. Vantomme. G. Langouche and the ISOLDE collaboration
Nuclear Instruments and Methods in Physics Research B 136-138 (1998) 744-750.

Lattice sites and stability of implanted Er in FZ and CZ Si. IS368
U. Wahl, J.G. Correia, G. Langouche, A. Vantomme and the ISOLDE collaboration
Materials Research Society Proceedings 486 (1998) 269-274.

Lattice sites and damage annealing of Er in low-dose implanted GaAs. Is368
U. Wahl, A. Vantomme, G. Langouche and the ISOLDE collaboration
Nuclear Instruments and Methods in Physics Research B 148 (1999) 492-406.

The influence of oxygen on the lattice sites of rare earths in silicon. IS368
U. Wahl, A. Vantomme, G. Langouche, J.G. Correia and the ISOLDE collaboration
Journal of Luminescence 80 (1999) 303-307.

Lattice location of implanted Cu in Si. IS368
U. Wahl, J.G. Correia, A. Vantomme, G. Langouche, and the ISOLDE collaboration
Physica B 273-274 (1999) 367-370.

Er-O clustering and its influence on the lattice sites of Er in Si. IS368
U. Wahl, J.G. Correia, J.P. Araújo, A. Vantomme, G. Langouche, and the ISOLDE collaboration
Physica B 273-274 (1999) 342-345.

Study of indium-defect interactions in diamond using 2-D CEEC. IS368
B.P. Doyle, E.J. Storbeck, U. Wahl, S.H. Connell, J.P.F. Sellschop, and the ISOLDE collaboration
Journal of Physics: Condensed Matter 12 (2000) 67-78.

Lattice location and stability of ion implanted Cu in Si. IS368
U. Wahl, A. Vantomme, G. Langouche, J.G. Correia, and the ISOLDE collaboration
Physical Review Letters 84 (2000) 1495-1498.

Emission channeling studies of Pr in GaN. IS368
U. Wahl, A. Vantomme, G. Langouche, J.P. Araújo, L. Peralta, J.G. Correia, and the ISOLDE collaboration
Journal of Applied Physics 88 (2000) 1319-1324.

Lattice location of implanted Cu in highly-doped Si. IS368
U. Wahl, A. Vantomme, G. Langouche, J.P. Araújo, L. Peralta, J.G. Correia, and the ISOLDE collaboration
Applied Physics Letters 77 (2000) 2142-2144.

Direct evidence for implanted Fe on substitutional Ga sites in GaN. IS368
U. Wahl, A. Vantomme, G. Langouche, J.G. Correia, L. Peralta, and the ISOLDE collaboration
Applied Physics Letters 78 (2001) 3217-3220.

Emission channeling studies of implanted ^{167m}Er in InP. IS368
U. Wahl, A. Vantomme, G. Langouche, J.P. Araújo, and the ISOLDE collaboration
Nuclear Instruments and Methods in Physics Research B 175-177 (2001) 262-267.

Lattice location of implanted Ag in Si. IS368
U. Wahl, J.G. Correia, A. Vantomme, and the ISOLDE collaboration
accepted for publication by Nuclear Instruments and Methods in Physics Research B.

Cadmium-related defects in silicon: electron-paramagnetic resonance identification. P83
W. Gehlhoff, A. Näser, M. Lang, G. Pensl
Mater. Sci. Forum, Vols. 258-263, 423-428 (1997).

Identification of a Donor State of Substitutional Cadmium in Silicon. P83
A. Näser, W. Gehlhoff, H. Overhof and R.A. Yankov
phys.stat.sol.(b), 210, 753 (1998).

Identification of Cadmium related centers in silicon. P83
Näser, W. Gehlhoff, H. Overhof
Physica B 273-274, 279-282 (1999)

Iridium-Related Deep-Levels in n-Type Silicon. IS357
J.Bollmann, S.Knack, J. Weber,
Physica Status Solidi (b), 222, 251-260
(2000)

Chemically selective laser ion source of manganese. IS359
V.N. Fedoseyev, K. Bätzner, R. Catherall, A.H.M. Evensen, D. Forkel-Wirth, O.C. Jonsson, E. Kugler, J. Lettry, V.I. Mishin, H.L. Ravn, G. Weyer, and the ISOLDE Collaboration:
Nucl. Instr. Meth. B 126 (1997) 88

Mössbauer spectroscopy of Fe in silicon with the novel laser-ionised $^{57}Mn^{+}$ ion beam at ISOLDE. IS359
G. Weyer, S. Degroote, M. Fanciulli, V.N. Fedoseyev, G. Langouche, V.I. Mishin, A.-M. Van Bavel, A. Vantomme, and the ISOLDE Collaboration:
Mat. Sci. Forum 258-263 (1997) 437

The electronic configuration of substitutional Fe in silicon. IS359
G. Weyer, A. Burchard, M. Fanciulli, V.N. Fedoseyev, H.P. Gunnlaugsson, V.I. Mishin, R. Sielemann, and the ISOLDE Collaboration:
Physica B 273-274 (1999) 363

Mössbauer spectroscopy at ISOLDE. IS359
G. Weyer and the ISOLDE Collaboration:
Hyp. Int. 129 (2000) 371

High temperature configurations of Fe in silicon. IS359
H.P. Gunnlaugsson, G. Weyer, M. Dietrich, V.N. Fedoseyev, V.I. Mishin, R. Sielemann, M. Fanciulli, and the ISOLDE Collaboration:
Proc. 2nd ENDEASD Workshop, Stockholm 2000, ed. C. Claeys, (IMEC, Leuven, 2000) p. 28

Detection of substitutional and interstitial Fe in silicon by Mössbauer spectroscopy. IS359
H.P. Gunnlaugsson, M. Dietrich, M. Fanciulli, K. Bharuth-Ram, R. Sielemann, G. Weyer, and the ISOLDE Collaboration:
Physica Scripta, in press

^{57}Fe Mössbauer study of radiation damage in ion implanted Si, SiGe, and SiSn. IS359
H.P. Gunnlaugsson, M. Dietrich, M. Fanciulli, K. Bharuth-Ram, R. Sielemann, G. Weyer, and the ISOLDE Collaboration:
Nucl. Instr. Meth. B 186 (2001) 55 H.P.

Detection of diffusional jumps of interstitial Fe in silicon by Mössbauer spectroscopy. IS359
Gunnlaugsson, M. Dietrich, M. Fanciulli, K. Bharuth-Ram, R. Sielemann, G. Weyer, and the ISOLDE Collaboration:
Physica B 308-310 (2001) 418

Charge state dependence of the diffusivity of interstitial Fe in silicon observed by Mössbauer spectroscopy. IS359
H.P. Gunnlaugsson, M. Dietrich, M. Fanciulli, K. Bharuth-Ram, R. Sielemann, G. Weyer, and the ISOLDE Collaboration:
subm. to Appl. Phys. Lett.

Radioactive Isotopes in Photoluminescence Experiments: Identification of Defect Levels. IS345
R. Magerle, A. Burchard, M. Deicher, T. Kerle, W. Pfeiffer and E. Recknagel,
Phys. Rev. Lett. 75 (1995) 1594

The role of hydrogen in low-temperature MOVPE growth and carbon doping of $In_{0.53}Ga_{0.47}As$ for InP-based HBT. IS345
A. Lindner, P. Velling, W. Prost, A. Wiersch, E. Kuphal, A. Burchard, R. Magerle,
M. Deicher and F.J. Tegude,
J. Crystal Growth 170 (1997) 287

First PAC Studies on the Hydrogen Diffusion in III-V Semiconductors. IS345
A. Burchard, M. Deicher, R. Magerle, A. Egenter, R. Spengler and D. Forkel-Wirth,
in: “Shallow-Level Centers in Semiconductors” ed. C.A.J. Ammerlaan and B. Pajot,
(World Scientific, Singapore, 1997) p. 185

First Microscopic Observation of Cadmium-Hydrogen Pairs in GaN. IS345
A. Burchard, M. Deicher, D. Forkel-Wirth, E.E. Haller, R. Magerle, A. Prospero and R. Stötzler,
Materials Research Symposium Proc. Vol. 449 (1997) p. 961

Solid-State Physics and PIAFE. IS345
D. Forkel-Wirth, A. Burchard, M. Deicher, R. Magerle and U. Köster,
in: "Research with Fission Fragments" eds. T. v. Egidy, F.J. Hartmann, D. Habs, K.E.G. Loebner, and H. Nifenecker (World Scientific, Singapore 1997) p. 293

Recovery of Structural Defects in GaN after Heavy Ion Implantation. IS345
C. Ronning, M. Dalmer, M. Deicher, M. Restle, M.D. Bremser, R.F. Davis and H. Hofsäss,
Materials Research Symposium Proc. Vol. 468 (1997) 407

Creation of Ga_{As} Antisites in GaAs by Transmutation of Radioactive $^{71}As_{As}$ to Stable $^{71}Ga_{As}$. P104
R. Magerle, A. Burchard, D. Forkel-Wirth and M. Deicher,
in: "Defects in Semiconductors 19", eds. G. Davies and M. H. Nazaré,
Materials Science Forum Vol. 258-263 (Trans Tech Publications 1997) p. 945

Implantation Doping and Hydrogen Passivation of GaN. IS345
A. Burchard, M. Deicher, D. Forkel-Wirth, E.E. Haller, R. Magerle, A. Prospero and A. Stötzler,
in: "Defects in Semiconductors 19", eds. G. Davies and M. H. Nazaré,
Materials Science Forum Vol. 258-263 (Trans Tech Publications 1997) p. 1099

Aceptor-Hydrogen Interaction in InAs. IS312, IS345
A. Burchard, J. G. Correia, M. Deicher, D. Forkel-Wirth, R. Magerle, A. Prospero and A. Stötzler,
in: "Defects in Semiconductors 19", eds. G. Davies and M. H. Nazaré,
Materials Science Forum Vol. 258-263 (Trans Tech Publications 1997) p. 1223

Microscopic study of the hydrogen diffusion in III-V semiconductors. IS345
A. Burchard, M. Deicher, D. Forkel-Wirth, M. Knopf, R. Magerle, A. Stötzler, V.N. Fedoseyev andV.I. Mishin,
Materials Research Symposium Proc. Vol. 513 (1998) p. 171

Electric Field Gradients of Acceptor-Donor Pairs in Semiconductors. IS345
A. Burchard, M. Deicher, V.N. Fedoseyev, D. Forkel-Wirth, R. Magerle, V.I. Mishin, D. Steiner, A. Stötzler, R. Weissenborn and Th. Wichert,
Hyperfine Interactions 120/121 (1999) 389

Annealing of Ion Implanted GaN. IS345
A. Burchard, E.E. Haller, A. Stötzler, R. Weissenborn and M. Deicher,
Physica B 273-274 (1999) 96

Identification of Ag and Cd Photoluminescence in ^{111}Ag Doped GaN. P104
A. Stötzler, R. Weissenborn and M. Deicher,
Physica B 273-274 (1999) 144

Identification of As, Ge and Se Photoluminescence in GaN Using Radioactive Isotopes. P104
A. Stötzler, R. Weissenborn and M. Deicher
Proc. MRS 1999 Fall Meeting, Symposium W: GaN and Related Alloys,
Materials Research Symposium Proc. Vol. 595 (2000) in press, and
MRS Internet J. Nitride Semicond. Res. 5S1 (2000) W12.9
(http://nsr.mij.mrs.org/5S1/W12.9/)

Photoluminescence characterization of Mg implanted GaN. P104
C. Ronning, H. Hofsäss, A. Stötzler, M. Deicher, E.P. Carlson, P.J. Hartlieb, T. Gehrke, P. Rajagopal and R.F. Davis
Proc. MRS 1999 Fall Meeting, Symposium W: GaN and Related Alloys,
Materials Research Symposium Proc. Vol. 595 (2000) in press, and
MRS Internet J. Nitride Semicond. Res. 5S1 (2000) W11.44
(http://nsr.mij.mrs.org/5S1/W11.44/)

Photoluminescence analysis of semiconductors using radioactive isotopes. IS357
M.O. Henry, M. Deicher, R. Magerle, E. McGlynn and A. Stötzler
Hyperfine Interactions 129 (2000) 443

Nuclear techniques in the study of thermodynamic parameters of defects in semiconductors. IS345, IS369
M. Deicher and Th. Wichert
in: *Mass and Charge Transport in Inorganic Materials. Fundamentals to Devices*. Part A, eds. P. Vincenzini and V. Buscaglia, Vol. 29 of Adv. Sci. Technol. (TECHNA Srl, Faenza, Italy, 2000) p. 449

Near-infrared photoluminescence in GaN doped with radioactive platinum. P104
A. Stötzler and M. Deicher
Appl. Phys. Lett., submitted

Studies of semiconductors. IS345, IS368, IS369, IS380
Th. Wichert and M. Deicher
Nuclear Physics A 693 (2001) 327

The influence of phosphorus, arsenic and antimony vapour ambients on the diffusion of zinc into gallium arsenide . IS362
G. Bösker, H.-G. Hettwer, A. Rucki, N.A. Stolwijk, H. Mehrer, W. Jäger, and K. Urban
Materials Chemistry and Physics 42**,** 68 - 71 (1995).

Use of zinc diffusion into GaAs for determining properties of gallium interstitials. IS362
G. Bösker, N.A. Stolwijk, H.-G. Hettwer, A. Rucki, W. Jäger, and U. Södervall
Phys. Rev. B 52**,** 11927 (1995).

Properties of Ga self-interstitials in GaAs investigated by in-diffusion of cadmium. IS362
G. Bösker, N.A. Stolwijk, U. Södervall, and W. Jäger
Defect and Diffusion Forum 143 - 147, 1109 (1997).

Effects of source composition on diffusion and solubility of Zn in gallium arsenide. IS362
H.-G. Hettwer, N.A. Stolwijk, and H. Mehrer
Defect and Diffusion Forum 143- 147, 1117 (1997).

Diffusion of Nitrogen from a Buried Doping Layer in Gallium Arsenide Revealing the Prominent Role of As Interstitials. IS362
G. Bösker, N.A. Stolwijk, H. Mehrer, J. V. Thordson, U. Södervall, and T. G. Andersson
Phys. Rev. Lett., Vol. 81 (61), 3443 (1998).

Arsenic diffusion in intrinsic Gallium Arsenide. IS362
G. Bösker, N.A. Stolwijk, H. Mehrer, A. Burchard, and U. Södervall
Mat. Res. Soc. Symp. Proc. Vol. 528, 347 (1998).

Diffusion of Cd in GaAs and its correlation with self-diffusion on the Ga sublattice. IS362
G. Bösker, N.A. Stolwijk, H. Mehrer, U. Södervall, and W. Jäger
J. Appl. Phys. 86 (1999) 791.

Transmission electron microscopy investigations of the defect formation during Zn-diffusion in GaP and GaSb. IS362
Ch. Jäger. W. Jäger, G. Bösker, J. Pöpping, and N.A. Stolwijk
in: Proc. Int. Conf. Microscopy of Semiconducting Materials, Oxford/UK (1999), Inst. Phys. Conf. Ser. No. 164 (1999) 73.

Self-diffusion on the arsenic sublattice in GaAs investigated by the broadening of buried nitrogen doping layers. IS362
N.A. Stolwijk, G. Bösker, J.V. Thordson, T. G. Andersson, U. Södervall, Ch. Jäger, and W. Jäger
Physica B 273 - 274 (1999) 685.

Ch. Jäger, W. Jäger, J. Pöpping, G. Bösker, and N.A. Stolwijk IS362
Proc. X Conf. Electron Microscopy of Solids, Warsaw-Serock, Poland, ed. by E. Jezierska and J. A. Kozubowski (1999) 45.

Implantation and Diffusion of ^{73}As in GaAs and GaP. IS362
G. Bösker, J. Pöpping, N.A. Stolwijk, H. Mehrer, U. Södervall, J.V. Thordson, T. G. Andersson, and A. Burchard
Hyperfine Interactions 129 (2000) 337.

Defect formation during Zn diffusion in GaP and GaSb. IS362
Ch. Jäger, W. Jäger, G. Bösker, J. Pöpping, and N.A. Stolwijk
Phil. Mag. A 80 (2000) 1.

Defect formation during Zn diffusion in GaP and GaSb. IS362
Ch. Jäger, W. Jäger, G. Bösker, J. Pöpping, and N.A. Stolwijk
Phil. Mag. A 80 (2000) 1.

Formation of metal precipitates and voids by zinc diffusion in GaP. IS362
Ch. Jäger, W. Jäger, J. Pöpping, G. Bösker, and N.A. Stolwijk
Journal of Electron Microscopy 48 (Suppl.) (2000) 1037.

Diffusion of Zn in gallium phosphide under defect-free phosphorus-rich conditions. IS362
J. Pöpping, N.A. Stolwijk, U. Södervall, Ch. Jäger, and W. Jäger
Physica B, in press

Acceptor-Hydrogen Complexes in InAs. IS345
D. Forkel-Wirth, N. Achtziger, A. Burchard, J.C. Correia, M. Deicher, J. Grillenberger, H. Gottschalk, T. Licht, U. Reislöhner, M. Rüb, M. Toulemonde, W. Witthuhn and the ISOLDE Collaboration
Materials Science Forum, Vol. 196-201 (1995) 963-968

Emission Channeling. IS342
H. Hofsäss,
Hyp. Int. 97/98 (1996) 247-283

Ion implanted impurities in GaN and AlN: lattice sites, annealing behavior and defect recovery. IS342
C. Ronning, M. Dalmer, M. Uhrmacher, M. Restle, U. Vetter, L. Ziegeler, H. Hofsäss,
T. Gehrke, K. Järrendahl, R.F. Davis,
J. Appl. Phys. 87 (2000) 2149

Combination of Emission Channeling, Photoluminescence and Mössbauer Spectroscopy to Identify Rare Earth Defect Complexes in Semiconductors. IS342
M. Dalmer , U. Vetter[a], M. Restle , A. Stötzler, H. Hofsäss , C. Ronning, V.V. Naicker,
M.K. Moodley, K. Bharuth-Ram and the ISOLDE-Collaboration,
Proc. 11th Int. Conf. on Hyperfine Interactions, Hyp. Int. 120/121 (1999) 347

Lattice Location and Luminescence Behavior of Rare Earth Elements Implanted in GaN. IS342
M. Dalmer, M. Restle, A. Stötzler, U. Vetter, H. Hofsäss, M.D. Bremser, C. Ronning,
R.F. Davis and ISOLDE Collaboration, in „Nitride Semiconductors, S. DenBaars, B. Meyer,
S. Nakamura, F. Ponce (eds.), Mat. Res. Soc. Proc. Vol. 482 (1998) 1021-1026

Li Ion Implantation Studies in GaN. IS342
M. Dalmer, M. Restle, C. Ronning, M. Sebastian, U. Vetter, H. Hofsäss, M.D. Bremser,
R.F. Davis, U. Wahl, K. Bharuth-Ram, and ISOLDE Collaboration,
J. Appl. Phys. 84 (1998) 3085

Perturbed Angular Correlation Measurements and Lattice Site Location of Br in GaAs. IS345
M. Wehner, M. Risse, R. Vianden, M. Dalmer, H. Hofsäss, M.C. Ridgeway, M. Petravic and ISOLDE Collaboration, Mater. Sci. For. 258-263 (1997) 899

Advances in electron emission channeling measurements in semiconductors. IS368
U. Wahl
Hyperfine Interactions 129 (2000) 349-370.

Emission channeling studies of implanted ^{167m}Er in InP. IS368
U. Wahl, A. Vantomme, G. Langouche, J.P. Araújo, and the ISOLDE collaboration
Nuclear Instruments and Methods in Physics Research B 175-177 (2001) 262-267.

Lattice Location Studies of Indium In Cr_2O_3. IS341
U. Vetter, M. Uhrmacher, D. Schwen, A. Lohstroh, H. Hofsäss and K.-P. Lieb, 12th Int. Conf. on Hyp. Int., Park City, Utah, USA, Aug. 13-17, 2001, Hyp. Int. (2002) to be published

Lattice site and diffusion of ion-implanted Li in as-grown and Se-rich ZnSe. IS341
K. Bharuth-Ram, M. Restle, H. Hofsäss, C. Ronning, U. Wahl, and ISOLDE Collaboration
Physica B 273 (1999) 875

Emission Channeling Studies of Defect Annealing in the Wide Band Gap Semiconductors ZnTe and ZnSe. IS341
K. Bharuth-Ram, H. Hofsäss, M. Restle, U. Wahl and the ISOLDE Collaboration, Nucl. Instr. Meth. B 156 (1999) 244

Li-Defect Reactions During Low Dose Ion Implantation of ^{8}Li into ZnSe Single Crystals. IS341
M. Restle , M. Dalmer, U. Wahl, H. Hofsäss and ISOLDE Collaboration, Mat. Res. Soc. Symp. Proc. 540 (1999)

Annealing Behaviour of ZnTe Investigated with ^{111m}Cd-Emission Channeling. IS341
K. Bharuth-Ram, M. Restle and H. Hofsäss, Nucl. Instr. Meth B 136 (1998) 751

Thermal Stability of Substitutional Ag in CdTe and ZnSe. IS341
S.G. Jahn, H. Hofsäss, M. Restle, C. Ronning, H. Quintel, K. Bharuth-Ram and U. Wahl, and the ISOLDE Collaboration, J. Cryst. Growth 161 (1996) 172

Lattice Sites of Li in CdTe. IS341
M. Restle, K. Bharuth-Ram, H. Quintel, C. Ronning, H. Hofsäss, S.G. Jahn and U. Wahl, and the ISOLDE Collaboration, J. Cryst. Growth 161 (1996) 168-171

Amorphization of ZnSe by Ion Implantation at Low Temperatures. IS341
S.G. Jahn, H. Hofsäss, M. Restle, C. Ronning, H. Quintel, K. Bharuth-Ram, and the ISOLDE-Collaboration, in Ion Beam Modification of Materials, eds. J.S. Williams, R.G. Elliman, M.C. Ridgway, (Elsevier, Amsterdam, 1996) p. 907-911

Implanted light dopants in ZnSe. P67
B. Ittermann, M. Füllgrabe, M. Heemeier, F. Kroll, F. Mai, K. Marbach, P. Meier, D. Peters, H. Thiess, G. Welker, H. Ackermann, H.-J. Stöckmann, W.-D. Zeitz, W. Geithner, S. Kappertz, S. Wilbert, R. Neugart, P. Lievens, U. Georg, M. Keim, and ISOLDE-Collaboration
Hyperfine Interact. 120/121, 403 (1999).

β-NMR in II-VI semiconductors. P67
B. Ittermann, M. Füllgrabe, M. Heemeier, F. Kroll, F. Mai, K. Marbach, P. Meier, D. Peters, G. Welker, W. Geithner, S. Kappertz, S. Wilbert, R. Neugart, P. Lievens, U. Georg, M. Keim, and ISOLDE-Collaboration
Hyperfine Interact. 129, 423--441, (2000).

Defect reactions of implanted Li in ZnSe observed by β-NMR. P67
F. Kroll, B. Ittermann, M. Füllgrabe, F. Mai, K. Marbach, D. Peters, W. Geithner, S. Kappertz, M. Keim, S. Kloos, S. Wilbert, R. Neugart, P. Lievens, U. Georg, and ISOLDE Collaboration
Physica B, in print (2001).

PAC investigation of ordered vacancy semiconductors of type $\square A^{II}B_2^{III}C_4^{VI}$. IS396
M.Dietrich, S.Unterricker, M.Deicher, A.Burchard, R.Magerle, W.Pfeiffer, D.Forkel-Wirth, I.M.Tiginyanu, N.A.Moldovyan and the ISOLDE, Hyperfine Interactions (C) 1 (1996) 242

Quadrupole interaction in defect chalcopyrite semiconductors studied by PAC. IS396
M.Dietrich, S.Unterricker, M.Deicher, A.Burchard, R.Magerle, W.Pfeiffer, D.Forkel-Wirth, I.M.Tiginyanu, N.A.Moldovyan and the ISOLDE-Collaboration, Cryst. Res. Technol. 31 (1996) 853

PAC-investigation of ternary semiconductors with chalcopyrite structure. IS396
S.Unterricker, M.Dietrich, A.Möller, R.Vianden, M.Deicher, R.Magerle, W.Pfeiffer, G.Böhm, L.Pasemann and the ISOLDE-Collaboration, Cryst. Res. Technol. 31 (1996) 761

Quadrupole interaction in chalcopyrite-structure semiconductors. IS396
S.Unterricker, M.Dietrich, G.Böhm, L.Pasemann, A.Möller, R.Vianden, M.Deicher, R.Magerle, A.Burchard, W.Pfeiffer, Hyperfine Interactions (C) 1 (1996) 238

TDPAC-investigations of the electric field gradient with ^{77}Br in ternary semiconductors. IS396
A.Möller, R.Vianden, S.Unterricker, M.Dietrich, D.Forkel-Wirth, Hyperfine Interactions (C) 1 (1996) 246

Disordering in defect chalcopyrites ? $A^{II}B^{III}_2C^{VI}_4$ studied by PAC. IS396
M.Dietrich, S.Unterricker, D.Degering, M.Deicher, R.Magerle, A.Burchard, D.Forkel-Wirth, I.M.Tiginyanu and the ISOLDE-Collaboration, Inst. Phys. Conf. Ser. No 152: Section E: Surfaces and Interfaces (1998) 781

Electric Field Gradients in Wurtzite - Type Semiconductors. IS396
M.Dietrich, J.Kortus, W.Cordts, S.Unterricker, phys. stat. sol. (b) 207 (1998) 13

The structure of ? $A^{II}B^{III}_2C^{VI}_4$ type defect chalcopyrites as investigated by PAC. IS396
S.Unterricker, M.Dietrich, D.Degering, J.Kortus, M.Deicher, R.Magerle, A.Burchard and the ISOLDE-Collaboration, Inst. Phys. Conf. Ser. No 152: Section E: Surfaces and Interfaces (1998) 777

Quadrupole Interaction in Ternary Chalcopyrite Semiconductors: Experiments and Theory. IS396
M. Dietrich, A. Burchard, D. Degering, M. Deicher, J. Kortus, R. Magerle, A. Möller, V. Samokhvalov, S. Unterricker, R. Vianden, Z. Naturforsch. 55 a, p. 256-260 (2000)

Local Probes in Magnetic Semiconductors – PAC Investigations. IS396
V. Samokhvalov, A. Richter, D. Degering, S. Unterricker, M. Dietrich, M. Deicher, I.M. Tiginyanu, Jap. J. Appl. Phys., vol. 39, suppl. 39-1, pp. 470-471 (2000)

Electric quadrupole interaction in the $CdIn_2S_4$ spinel compound studied by ^{111}In(^{111}Cd) - PAC: experiment and theory. IS396
I.I. Burlakov, V. Samokhvalov, S. Unterricker, M. Dietrich, and V.E. Tezlevan, phys. stat. sol. (b) 221, R11 (2000).

Response of the Electric Field Gradient in Ion implanted BaTiO3 to an External Electric Field. IS396
M. Dietrich, J. Bartels, M. Deicher, K. Freitag, V. Samokhvalov and S. Unterricker, Mat. Res. Soc. Symp. Vol. 655 (2001) CC10.11.1

Ferromagnetic semiconductors studied by hyperfine interaction of nuclear probes. IS396
S. Unterricker, V. Samokhvalov, I. Burlakov, D. Degering, M. Dietrich, M. Deicher and the ISOLDE Collaboration, Contribution to 12th International Conference on Hyperfine Interaction, Park City, Utah, August 12-17, 2001, accepted for Hyperfine Interactions (2002).

Atomic Configurations of Group V Acceptors in ZnSe, ZnTe, and CdTe. IS369
V. Ostheimer, A. Jost, T. Filz, St. Lauer, H. Wolf, and Th. Wichert
Appl. Phys. Lett. 69 (1996) 2840

Passivation of shallow dopants in II-VI Semiconductors . IS369
H. Wolf, T. Filz, J. Hamann, A. Jost, V. Ostheimer, and Th. Wichert
in Shallow Level Centers in Semiconductors, edited by C.A.J. Ammerlaan and B. Pajot, World Scientific, Singapore, (1997) 123

Defect Structures in Heavily In Doped II-VI Semiconductors. IS369
V. Ostheimer, T. Filz, J. Hamann, St. Lauer, D. Weber, H. Wolf, and Th. Wichert
Materials Science Forum 258-263 (1997) 1341

Hydrogen-related Photoluminescence in CdTe. IS369
J. Hamann, D. Blaß, A. Burchard, C. Casimir, M. Deicher, T. Filz, R. Magerle, V. Ostheimer, C. Schmitz, H. Wolf, and Th. Wichert
J. Cryst. Growth 184/185 (1998) 1147

Hydrogen Related Photoluminescence in CdTe. IS369
J. Hamann, D. Blaß, C. Casimir T. Filz, V. Ostheimer, C. Schmitz, H. Wolf, Th. Wichert, A. Burchard, M. Deicher, and R. Magerle
Appl. Phys. Lett. 72 (1998) 554

Identification of Ag-Acceptor Related Photoluminescence in ^{111}Ag Doped CdTe. IS369
J. Hamann, A. Burchard, M. Deicher, T. Filz, V. Ostheimer, C. Schmitz, H. Wolf, Th. Wichert, and ISOLDE Collaboration
Appl. Phys. Lett. 72 (1998) 3029

The Incorporation and Complex Formation of Ag Acceptors in CdTe. IS369
H. Wolf, T. Filz, J. Hamann, V. Ostheimer, S. Lany, Th. Wichert, M. Deicher, A. Burchard, and ISOLDE Collaboration;
Mat. Res. Soc. Symp. Proc. 510 (1998) 337

Magneto-Optical Properties of a Hydrogen-Related Defect in CdTe. IS369
J. Hamann, L. Worschech, D. Blaß, C.Y. Hu, T. Filz, W. Ossau, V. Ostheimer, C. Schmitz, H. Wolf, and Th. Wichert;
Phys. Stat. Sol. (b) 210 (1998) 513

Doping of CdTe with radioactive ^{111}In during MOCVD growth. IS369
V. Ostheimer, T. Filz, J. Hamann, St. Lauer, Ch. Schmitz, D. Weber, H. Wolf, and Th. Wichert;
J. Cryst. Growth 198-199 (1999) 1184

Perturbed Angular Correlation Studies of Defects. IS369
Th. Wichert;
in: "Identification of Defects in Semiconductors", edited by M. Stavola, Semiconductors and Semimetals 51B (1999) 297, Academic Press, San Diego, CA

Luminescence and Influence of Defect Concentration on Excitons in ^{197}Hg/^{197}Au doped CdTeJ. IS369
Hamann, A. Burchard, M. Deicher, T. Filz, V. Ostheimer, F. Strasser, H. Wolf, ISOLDE Collaboration, and Th. Wichert;
Physica B 273-274 (1999) 870

Defect Complexes Induced by Diffusion of Group I Acceptors into CdTe. IS369
H. Wolf, T. Filz, J. Hamann, S. Lany, V. Ostheimer, and Th. Wichert;
Physica B 273-274 (1999) 843

Electric field gradients of acceptor–donor pairs in semiconductors. IS369
A. Burchard, M. Deicher, V.N. Fedoseyev, D. Forkel-Wirth, R. Magerle, V.I. Mishin, D. Steiner, A. Stötzler, R. Weissenborn, Th. Wichert, ISOLDE-Collaboration
Hyperfine Interactions 120/121 (1999) 389

Identification of Ag-Acceptors in ^{111}Ag/^{111}Cd doped ZnTe and CdTe. IS369
J. Hamann, A. Burchard, M. Deicher, T. Filz, S. Lany, V. Ostheimer, F. Strasser, H. Wolf, ISOLDE Collaboration, and Th. Wichert
J. Cryst. Growth 214/215 (2000) 207

Defect Complexes Formed with Ag Atoms in CdTe, ZnTe, and ZnSe. IS369
H. Wolf, T. Filz, V. Ostheimer, J. Hamann, S. Lany, ISOLDE Collaboration, and Th. Wichert
J. Cryst. Growth 214/215 (2000) 967

Investigation of Group V Acceptors in CdTe: Ab initio Calculation of Lattice Relaxation and the Electric Field Gradient. IS369
Stephan Lany, Peter Blaha, Joachim Hamann, Volker Ostheimer, Herbert Wolf, and Thomas Wichert
Phys. Rev. B 62 (2000) R2259

Defect-Induced Bound-Exciton Lines in Hydrogen-Doped CdTe: Zeeman Spectroscopy. IS369
J. Hamann, L. Worschech, S. Lany, W. Ossau, V. Ostheimer, C. Schmitz, H. Wolf, and Th. Wichert
Proc. 25th Int. Conf. Phys. Semicond., N. Miura and T. Ando eds., Springer Berlin Heidelberg (2001) 1439

Photoluminescence Study of II-VI Semiconductors by Using Radioactive ^{71}As Dopants. IS369
S. Lany, J. Hamann, ISOLDE Collaboration, V. Ostheimer, H. Wolf, and Th. Wichert
Physica B 302/303 (2001) 114

The Strange Diffusivity of Ag Atoms in CdTe. IS369
H. Wolf, M. Deicher, V. Ostheimer, A. Rodriguez Schachtrup, N.A. Stolwijk, Th. Wichert, ISOLDE Collaboration
Physica B 308-310 (2002) 963

Vacancies in CdTe: Experiment and theory. IS369
S. Lany, V. Ostheimer, H. Wolf, Th. Wichert
Physica B 308-310 (2002) 958

Defect identification by means of EFG calculation. IS369
S. Lany, V. Ostheimer, H. Wolf, Th. Wichert, ISOLDE Collaboration
Physica B 308-310 (2002) 980

Calculated electric field gradients and electronic properties of acceptors in CdTe. IS369
S. Lany, V. Ostheimer, H. Wolf and Th. Wichert
accepted for publication in Hyperfine Int. (2002)

Identification of Defects in Semiconductors via their Electric Field Gradients. IS369
Th. Wichert and St. Lany
accepted for publication in Hyperfine Int. (2002)

Incorporation of the Donor In in Nanocrystalline ZnO. IS369
Th. Agne, Z. Guan, X.M. Li, H. Wolf, Th. Wichert
accepted for publication in Phys. Stat. Sol. B 229 (2002)

Nitrogen-acceptor pairs in n-type 4H-SiC observed by the perturbed angular correlatioon spectroscopy . IS325
Th. Licht, N. Achtziger, D. Forkel-Wirth, U. Reislöhner, M. Rüb, M. Uhrmacher, W. Witthuhn and ISOLDE Collaboration
Inst. Phys. Conf. Ser. No. 142 (1996) 461-464

Structural and electrical investigation of implantation damage annealing in CdTe . IS325
N. Achtziger, J. Bollmann, Th. Licht, B. Reinhold, U. Reislöhner, J. Röhrich, M. Rüb, M. Wienecke, W. Witthuhn and ISOLDE Collaboration
Semicond. Sci. Technol. 11 (1996) 947-951

Hafnium, Cadmium and Indium Impurities in 4H-SiC observed by Perturbed Angular Correlation Spectroscopy. IS325
Th. Licht, N. Achtziger, D. Forkel-Wirth, K. Freitag, J. Grillenberger, M. Kaltenhäuser, U. Reislöhner, M. Rüb, M. Uhrmacher, W. Witthuhn and ISOLDE Collaboration
Diamond and Related Materials 6 (1997) 1436-1439

Investigations on implantation doping of wide-bandgap II-VI compounds using radioactive dopants. IS325
M. Wienecke, B. Reinhold, J- Röhrich, J. Bollmann, N. Achtziger, U. Reislöhner, W. Witthuhn, S. Hermann and The ISOLDE Collaboration
J. Phys. D: Appl. Phys. 32 (1999) 291-297

Chemisorption of isolated Br atoms on Si(100)2x1 studied by PAC. IS318
J. Lohmüller, H. H. Bertschat, H. Granzer, H. Haas, G.Schatz, W.-D. Zeitz, and the ISOLDE - Coll.,
Surface Science 360, 213 (1996).

PAC investigations of $^{77}Br \rightarrow {}^{77}Se$ on silicon surfaces. IS318
J. Lohmüller, H. H. Bertschat, H. Granzer, H. Haas, G.Schatz, W.-D. Zeitz,
and the ISOLDE - Coll.,
Hyp. Int. 97/98, 203 (1996).

Magnetic Hyperfine Fields at Se Adatoms on Ni Surfaces. IS318
H. Granzer, H. H. Bertschat, H. Haas and W.-D. Zeitz, J. Lohmüller, G. Schatz,
and the ISOLDE - Coll.,
Phys. Rev. Lett. 77, 4261 (1996).

New Approach for Range Measurements of Induced Magnetic Interactions in Pd. IS318
H. H. Bertschat, H. Granzer, H. Haas, R. Kowallik, S. Seeger, W.-D. Zeitz,
and the ISOLDE - Coll.,
Phys. Rev. Lett. 78, 342 (1997).

Static Magnetic Hyperfine Fields in Magnetically Polarized Pd. IS318
H. H. Bertschat, H.-H. Blaschek, H. Granzer, K. Potzger, S. Seeger, W.-D. Zeitz,
H. Niehus, A. Burchard, D. Forkel-Wirth, and ISOLDE – Collaboration,
Phys. Rev. Lett. 80, 2721 (1998).

Correlation between local magnetic and structural properties at the Ni/Pd interface. IS318
K. Potzger, H. H. Bertschat, A. Burchard, D. Forkel-Wirth, H. Granzer, H. Niehus,
S. Seeger, W.-D. Zeitz, and ISOLDE – Collaboration,
Nucl. Instr. Meth. B146, 618 (1998).

Interface Magnetism Using Radioactive Atoms. IS318
H. H. Bertschat,
Journal of Magnetism and Magnetic Materials 198-199, 636 (1999).

Nuclear stimulated desorption of isolated cadmium atoms from structured surfaces. IS318
Y. Ashkenazy, I. Kelson, H. H. Bertschat, K. Potzger, A. Weber, W.-D. Zeitz, and ISOLDE – Collaboration,
Surface Science Letters, 442, L1001 (1999).

Surface and Interface Studies with ASPIC. IS375
H. H. Bertschat, H. Granzer, K. Potzger, S. Seeger, A. Weber, W.-D. Zeitz,
Doris Forkel-Wirth, and the ISOLDE Collaboration,
Hyperfine Interactions, 129, 475 (2000).

Radioactive ions for solid state investigations at magnetic surfaces and interfaces. IS375
H. H. Bertschat, K. Potzger, A. Weber, and W.-D. Zeitz,
to be published in European Physical Journal A.

Temperature dependence of electric-field gradients at isolated Se adatoms on (001) and (111) surfaces and derived adatom distances. IS375
A.Weber, K. Potzger, H. Granzer, H. H. Bertschat, W.-D. Zeitz,
M. Dietrich, and B. Lindgren,
Phy. Rev. B64, 081404 (2001), Rapid Communication.

Coordination-number dependence of magnetic hyperfine fields at ^{111}Cd on Ni surfaces. IS375
K. Potzger, A. Weber, H. H. Bertschat, W.-D. Zeitz, and M. Dietrich,
submitted to PRL

Local Oxygen and Point Defects Probing in Hg-1201 High-T_C Superconductors. IS360
J.P. Araújo, J.G. Correia, S.M. Loureiro, P. Toulemonde, S. Le Floch, P. Bordet, J. J. Capponi, W.Tröger, B. Ctortecka, H.Haas, R. Gatt, J.G. Marques, J.C.Soares,
Physica C 341-348 (2000) 1969-1972.

Electron-Gamma Perturbed Angular Correlation Studies on High-T_C Superconductors. IS360
J.G. Correia, J.P. Araújo, J.G. Marques, A.R. Ramos, A.A. Lourenço, V. Amaral, V. Galindo, J.P. Senateur , F. Weiss, U. Wahl, A.A. Melo, J.C. Soares, J.B. Sousa, and the ISOLDE Collaboration, Hyperfine Interactions 129 (2000) 461-473

Local Oxygen Probing in the $HgBa_2CuO_{4+\delta}$ high-T_C Superconductor. IS360
J. G. Correia, J.P. Araújo, S.M. Loureiro, P. Toulemonde, S. Le Floch, P. Bordet, J. J. Capponi, R. Gatt, W.Tröger, B. Ctortecka, T. Butz, H.Haas, J. G. Marques, J.C. Soares,
Physical Review B 61 (2000) 11 769, 11 775

Electron-Gamma PAC: New Possibilities for NQI Studies . IS360
J.G. Correia, J.P. Araújo, J.G. Marques, A.R. Ramos, A.A. Melo, J.C. Soares, and the ISOLDE Collaboration,
Zeitschrift für Naturforschung 55a (2000) 3

Stability and Diffusion Studies of Hg Implanted $YBa_2Cu_3O_{6+x}$. IS360
J.P. Araújo, J.G. Correia, U. Wahl, J.G. Marques, E. Alves, V.S. Amaral, A.A. Lourenço, V. Galindo, T. von Papen, J.P. Senateur, F. Weiss, A. Vantomme, G. Langouche, A.A. Melo, M.F. da Silva, J.C. Soares, J.B. Sousa, and the ISOLDE Collaboration,
Nuclear Instruments and Methods B148, (1999) 807-812.

Stability Studies of Hg Implanted $YBa_2Cu_3O_{6+x}$. IS360
J.P. Araújo, J.G. Correia, U. Wahl, J.G. Marques, E. Alves, V.S. Amaral, A.A. Lourenço, V. Galindo, T. von Papen, J.P. Senateur, F. Weiss, A. Vantomme, G. Langouche, A.A. Melo, M.F. da Silva, J.C. Soares, J.B. Sousa, and the ISOLDE Collaboration,
Nuclear Instruments and Methods B147, (1998) 244-248

High-Tc Superconductors Studies with Radioactive Ion Beams at ISOLDE. IS360
J.G. Correia, and the IS360 Collaboration,
OECD/Nuclear Energy Agency report, on the OECD/NEA Workshop on Ion and Slow Positron Beam, September 1998, Costa da Caparica, Portugal

Microscopic Studies of Radioactive Hg Implanted in $YBa_2Cu_3O_{6+x}$ Superconducting Thin Films. IS360
V.S.Amaral, J.G. Correia, A.A. Lourenço, J.G. Marques, J.A. Mendes, M.A. Baptista, J.P. Araújo, J.M. Moreira, J.B.Sousa, E. Alves, M.F. da Silva, J.C. Soares and the ISOLDE Collaboration, Journal of Magnetism and Magnetic Materials 177-181 (1997) 511

^{80m}Br/^{80}Br - A new electron-gamma PAC Probe. IS360
J.G. Correia, H. Haas, J.P. Araujo, J.G. Marques, A.A. Melo, J.C. Soares and the ISOLDE collaboration
accepted by Hyperfine Interactions

Surface quality studies of high-Tc superconductors of the Hg-, Tl- and Hg_xT_{l-x}-families: RBS and resonant C and O backscattering studies. IS360
A. Vantomme, E. Alves, J.G. Correia, I. Bryntse, Lars-G. Johansson, S.M. Loureiro, S. Lefloch, P. Toulemonde, P. Bordet and C. Bougerol-Chaillout
accepted by Nuclear Instruments and Methods in Physics Research B.

Lattice site location of Hg implanted $YBa_2Cu_3O_{6+x}$. IS360
J.P. Araújo, U. Wahl, J.G. Correia, A.A. Lourenço, V. Galindo, T. von Papen, J.P. Senateur, F. Weiss, A. Vantomme, G. Langouche,, and the ISOLDE Collaboration,
in preparation to PRB.

Dependence of the Electric Field Gradient of Ir in Fe on the Direction of Magnetization with respect to the Crystallographic Axes. IS314
G. Seewald, E. Hagn, E. Zech, D. Forkel-Wirth, A. Burchard and ISOLDE Collaboration
Phys. Rev. Lett. 78 (1997) 1795-1798

Experimental Evidence for a Large Collinear Electric Field Gradient of Ir in hcp-Co. IS314
G. Seewald, B. Hinfurtner, E. Hagn, E. Zech, D. Forkel-Wirth, R. Eder and ISOLDE Collaboration
Phys. Rev. Lett. 80 (1998) 3638-3641

Spin-Orbit Electric Field Gradient in Cubic Ferromagnets: Strong Magnetization-Direction Dependence of the Field Gradient Distribution. IS314
G. Seewald, E. Hagn, E. Zech, R. Kleyna, M. Voss, D. Forkel-Wirth, A. Burchard and ISOLDE Collaboration
Phys. Rev. Lett. 82 (1999) 1024-1027

Electric Quadrupolar Contribution to the Nuclear Spin-Lattice Relaxation of Ir in Fe. IS314
G. Seewald, E. Zech, H.J. Koerner, D. Borgmann, M. Dietrich and ISOLDE Collaboration
Phys. Rev. Lett. (2002), in press

Hyperfine fields at Cd site on $La_{0.67}Cd_{0.25}MnO_3$ CMR manganites. IS390
J.P. Araújo, J.G. Correia, V.S. Amaral, P.B. Tavares, F. Lencart-Silva, A.A.C.S. Lourenço, J.B. Sousa, J.M. Vieira, J.C. Soares , 133 (2001) pags. 89-94

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