Proposal to the ISC

Direct measurement of DX-center related
lattice relaxations in Al$_x$Ga$_{1-x}$As compounds

Konstanz$^1$ - Bonn$^2$ Collaboration

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Donor impurities from elements of group IV and VI form localized electronic states, so-called DX centers, in AlGaAs and other semiconductors. One of the well known effects related to DX-centers is the persistent photoconductivity. In spite of extensive studies, the microscopic structure of the DX center is still a matter of controversy. The direct determination of the donor lattice sites and their microscopical surrounding is a crucial point in understanding the relation of microscopic structure to the localized electronic state of the DX-center.

It is proposed to implant radioactive group VI elements \(^{73}\text{Se}\) (from \(^{73}\text{Br}\)) and \(^{118}\text{Te}\) (from \(^{118}\text{Xe}\)) into \( \text{Al}_x\text{Ga}_{1-x}\text{As} \) of different mole fractions \(x\) and to determine (i) the lattice sites of Te and Se impurities by emission channeling of decay positrons and electrons and (ii) the local structure of Se impurities using the perturbed \( \gamma-\gamma \) angular correlation technique (PAC). The appearance of the DX center shall be checked by electrical measurements. We request 16 shifts of \(^{73}\text{Br}\) and 8 shifts of \(^{118}\text{Xe}\).
Setup for on-line emission channeling measurements at ISOLDE

(1) Sample mounted on goniometer; (2) Cooling device; (3) Collimator;
(4) Detectors; (5) Beam line; (6) Lead shielding; (7) Collimator;
The DX-center in III-V semiconductors

Group IV elements such as Si and Sn replacing Ga(Al), or group VI elements like S, Se and Te replacing As form deep donors known as DX-centers in AlxGa1-xAs alloys and other semiconductors. DX centers have been extensively studied for over a decade, since they exhibit unusual and interesting electrical and optoelectronic properties and seriously affect the performance of electronic devices. The microscopic structure of the deep donor level, however, remains controversial up to now.

The current status of research on DX centers in III-V semiconductors was recently reviewed in an article by Mooney [1]. It turns out that DX centers are characterized by the following features: (i) the existence of an energy barrier for capture and emission of electrons which determine the transition rates of electrons to and from the DX center. For Te or Se doped AlxGa1-xAs this barrier is about 28 meV for emission and 14 meV for capture resulting in exceedingly small electron capture cross sections at low temperatures; (ii) the large binding energy of up to 180 meV depending on the alloy composition. In Si doped AlxGa1-xAs for example the DX-level drops below the bottom of the conduction band for x > 0.22 and then controls the conductivity of the material; (iii) The large difference between optical ionization energy (0.85 eV for Te doped AlxGa1-xAs) and thermal ionization energy which can be most naturally explained by assuming a large lattice relaxation mechanism.

As a consequence of these features the well known effect of persistent photoconductivity (PPC) is observed: at low temperatures, when thermally activated capture and emission processes become unlikely, photoexcitation increases the conductivity which remains for hours after illumination [2].

There have been many efforts to explain the physical origin of the DX center, however, most of the experimental results obtained so far are from studies of the electrical and optical properties of the DX center. These data do not give direct information about the microscopic structure of the DX level, i.e. the lattice position of the donor atoms and the structure of the immediate surrounding. As a consequence, several different models for the DX center were proposed. In the first model proposed by Lang et al. [3], which seems to be no longer accepted, a defect complex consisting of the donor atom and possibly an As vacancy was introduced to explain a large lattice relaxation. It is now generally accepted that the DX is an intrinsic feature of n-type dopants. Currently two fundamentally different approaches to the microscopic model of the DX center are discussed, the large lattice relaxation (LLR) models and the small lattice relaxation (SLR) models.

Recent LLR models assume that the capture of a second electron decreases the energy of the deep level, forming a so called negative U center. This happens when the increased energy due to the repulsion of the two electrons is offset by an energy decrease due to a large lattice relaxation [4,5]. In other LLR models the lattice relaxation is explained for example by a Jahn-Teller effect [6]. A recent SLR model is based on the assumption that the DX center is linked to the L minimum of the AlxGa1-xAs conduction band and causes only weak rearrangements of the surrounding lattice [7].
Experimental Techniques

The goal of our proposed experiments is to prove the validity of the LLR models by measuring directly the donor lattice location as well as the microscopical surrounding of donor atoms.

The direct measurement of a lattice relaxation of a donor atom with conventional lattice location techniques, like Rutherford backscattering spectroscopy (RBS) - channeling, is difficult because of typical donor concentrations below $10^{19}$ cm$^{-3}$. Since RBS-channeling requires heavy impurity atoms it can only be applied to Te doped Al$_x$Ga$_{1-x}$As samples [8]. Mössbauer spectroscopy at $^{129}$mTe implanted Al$_{0.36}$Ga$_{0.64}$As has revealed a quadrupole split line indicating a fraction of Te on non-cubic axially symmetric sites which were attributed to the DX center [9]. However the interpretation of these experiments in terms of a relaxation of the donor atoms is ambiguous.

**Emission Channeling** is a lattice location technique which was successfully applied at ISOLDE to determine impurity lattice sites in metals and semiconductors after very low dose implantations [10,11]. In this technique, radioactive impurities are implanted into the samples and the channeling and blocking effects of emitted decay electrons, positrons or alpha particles are measured for different crystallographic directions. From this, the distribution of impurity lattice sites can directly be derived. The main advantages of the technique are: (i) the low impurity concentrations necessary, typically $10^{17}$ cm$^{-3}$; (ii) no additional radiation damage due to an external analyzing beam; (iii) many suited isotopes can be used as probe atoms. Therefore, emission channeling appears to be the ideal technique to investigate the donor lattice sites related to DX centers. Suited candidates as radioactive donors in Al$_x$Ga$_{1-x}$As are $^{73}$Se ($t_{1/2} = 7.1$ h), emitting positrons with E < 1.3 MeV as well as 55 keV conversion electrons in the decay to $^{73}$As, and $^{118}$Te ($t_{1/2} = 6$ d), emitting positrons with E < 2.7 MeV during the decay to $^{118}$Sn.

**Perturbed angular correlation** (PAC) is a technique which, after being well established as a tool for defect studies in metals, was also successfully applied at ISOLDE in the previous years to study dopant-defect complexes in semiconductors [12]. The PAC method measures the nuclear spin precession frequencies that are caused by the electric field gradient (EFG) arising from asymmetries in the crystal environment of the PAC probe atom. The following information can be obtained from a PAC measurement: (i) the fraction of probe atoms exposed to a particular unique EFG; (ii) the quadrupole interaction strength associated with that EFG; (iii) the symmetry of the EFG tensor; (iv) the orientation of the EFG tensor components with respect to the crystal lattice; (v) the dynamics of fluctuating EFG′s, providing information about defect mobilities.
Due to the required nuclear properties PAC is restricted to several suited probe nuclei, from which $^{111}$In and $^{111}$mCd are the most commonly used. However, recent improvements in the measuring technique [13] allows the use of PAC probes with less favorable nuclear properties but the necessary elemental characteristics for studies in semiconductors. For the proposed experiments it is crucial that with the $^{73}$Se a donor probe in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ has become available [14,15].

From both emission channeling and PAC measurements we expect to derive a microscopical model of the atomic structure around Se and Te in $\text{Al}_x\text{Ga}_{1-x}\text{As}$.

**Proposed experiments**

It is planned to implant $^{118}$Te and $^{73}$Se at room temperature into $\text{Al}_x\text{Ga}_{1-x}\text{As}$ samples of different mole fractions $x$ at doses of about $10^{12}$ to $5\times10^{13}$ cm$^{-2}$ (sample size about 5x5 mm$^2$). Some of the samples are pre-doped with stable Se or Te in order to obtain the required donor concentrations without introducing too much implantation damage. Samples are then annealed using rapid thermal annealing to remove implantation damage. Emission channeling and PAC measurements are performed at different temperatures (room temperature and 77K) as well as before and after illumination of the samples. Since it is known that most of the Te or Se donor atoms contribute to the DX centers for $x > 0.3$ we expect sufficiently large channeling and PAC signals.

From emission channeling measurements the lattice location of Te and Se shall be determined. From this a possible interstitial fraction of Te or Se impurities can be easily identified, thus clarifying whether the LLR-model is valid or not. For the case of $^{73}$Se, PAC can determine the fraction of unperturbed substitutional and possibly non-substitutional or defect-related impurities. Furthermore from the asymmetry of an observed EFG the symmetry of the microscopical surrounding can be determined.

In addition, electrical measurements at low temperatures are planned to check the existence of DX centers in the prepared samples.

To complete the proposed measurements under the various experimental conditions outlined above we estimate about 16 samples for each isotope.

**Experimental Requirements**

All experiments simply require the collection of radioactive isotopes at room temperature using standard ion sources (Xe source for implantation of $^{118}$Te, Br-source for implantation of Se). A collection-chamber which can be connected to the ISOLDE beam-line already exists.

Emission channeling measurements can be performed off-line using a channeling setup at ISOLDE as well as setup in Konstanz, one of them equipped with position sensitive detectors for positrons.
Necessary treatments of the samples and the PAC measurements can be performed off-line at Bonn and at the 4-detector setup at ISOLDE.

Request of beamtime

For channeling measurements with $^{118}$Xe/$^{118}$Te a collection time of about 0.5 shifts is needed to prepare one sample. Therefore we request 8 shifts of collection time. This number may be split into smaller blocks.

For channeling and PAC measurements using $^{73}$Se we also assume a collection time of about 0.5 shifts per sample, corresponding to a total request of 16 shifts.

References
