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Emission channeling studies of implanted ^{167m}Er in InP

U. Wahl, A. Vantomme, G. Langouche
Instituut voor Kern- en Stralingsfysica,
University of Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium

J.P. Araújo
IFIMUP, University of Porto, P-4150 Porto, Portugal

The ISOLDE collaboration
CERN-PPE, CH-1211 Genève 23, Switzerland

Abstract

We have used conversion electron emission channeling to determine the lattice location of ^{167m}Er ($t_{1/2}=2.28$ s) in InP after 60 keV room temperature implantation of ^{167}Tm ($t_{1/2}=9.25$ d) at a dose of $6.8 \times 10^{12} \text{ cm}^{-2}$. Following annealing at temperatures above the major recovery step of the implantation damage at 100-150°C, we observe around 75% of Er on substitutional In sites. A smaller fraction of Er (7%) is found on substitutional P sites, the remainder on random sites. Annealing the unprotected InP crystal at temperatures above 250°C in vacuum causes a decrease in the channeling effects.

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Corresponding author:

Ulrich Wahl

Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven,
Celestijnenlaan 200 D, B-3001 Leuven, Belgium

e-mail: ulrich.wahl@fys.kuleuven.ac.be

phone: ++32-16-327617

fax: ++32-16-327985

Introduction

Erbium doped InP shows luminescence at a wavelength of 1.54 μm [1-9], which is an interesting feature for infrared optoelectronic devices. Incorporation of Er in InP has been reported from both ion implantation [1-8] and doping during growth by metalorganic vapour phase epitaxy (MOVPE) [9]. An interesting aspect of the InP:Er system is the fact that its electroluminescence (EL) intensity is thermally stable and only slightly quenched at room temperature. This is in contrast to, e.g., the photo- and electroluminescence of Er in Si, but also to the Er photoluminescence (PL) in InP itself [3,4]. In order to explain this behaviour, it has been suggested that Er can exist in different configurations in InP. The absence of pronounced EL quenching was attributed to Er atoms occupying sites where they can be effectively excited via direct electron impact. On the other hand, the PL should be mainly caused by Er centers which are excited less efficiently by electron-hole recombination processes [3,4]. In that respect it is interesting to study possible lattice sites of implanted Er in InP. Substitutional In sites have been considered theoretically and are assumed to be the most likely occupied lattice positions of rare earth atoms in the 3+ ionization state [10]. Among the various rare earth doped InP systems only the lattice site of implanted Yb has been investigated previously by direct lattice location methods. Using the Rutherford backscattering (RBS) channeling technique, a 50% reduction in the backscattering yield of Yb was observed along the $\langle 100 \rangle$ direction [5-8]. However, the investigation of the axial $\langle 100 \rangle$ channeling alone does not allow one to discriminate, for instance, substitutional from tetrahedral interstitial sites or provide sublattice sensitivity and hence is not sufficient to unambiguously derive the lattice location.

In order to carry out detailed lattice location studies of implanted Er in InP, we have applied conversion electron emission channeling [11] from the short-lived isotope ^{167m}Er ($t_{1/2}=2.28$ s). This excited nuclear state is populated as a consequence of the radioactive decay of the isotope ^{167}Tm (9.25 d) and de-excites

into the ^{167}Er ground state by the emission of conversion electrons. The emitted electrons experience channeling or blocking effects along low-index crystal directions. This leads to an anisotropic electron emission yield from the crystal surface which depends in a characteristic way on the lattice sites occupied by the emitter atoms. Previously we have used this method to study the lattice sites of Er in Si and GaAs [12-14].

Experimental

The sample used in our experiment was a $\langle 111 \rangle$ -cut undoped n -InP single crystal (resistivity 0.09-0.04 Ωcm , carrier concentration $n=1.7\text{-}4.5 \times 10^{16} \text{ cm}^{-3}$). The radioactive isotope ^{167}Tm was implanted at 60 keV by means of the ISOLDE facility at CERN, using a 1 mm beam spot, 7° tilted implantation and a dose of $6.8 \times 10^{12} \text{ cm}^{-2}$. These parameters correspond to a $[\text{Tm}+\text{Er}]$ peak concentration of $2.7 \times 10^{18} \text{ cm}^{-3}$ at a depth of 236 Å with a straggling of 99 Å. Following room temperature implantation the sample was annealed capless in vacuum at 10^{-6} mbar. In order to detect the angular-dependent emission yield of the 150, 199 and 206 keV conversion electrons emitted by $^{167\text{m}}\text{Er}$ we used the position and energy sensitive detection system described in Refs. [12,13].

Results and discussion

Figs. 1(a)-(d) show the normalized $^{167\text{m}}\text{Er}$ conversion electron emission yields around the $\langle 111 \rangle$, $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 211 \rangle$ directions following annealing at 100°C and 150°C for 10 minutes. Emission channeling effects are visible along all axial and planar directions, which is clear evidence that the majority of $^{167\text{m}}\text{Er}$ atoms occupy substitutional sites. In order to analyze the lattice location more precisely we fitted theoretical emission patterns for different sites to the experimental data. The fitting procedure applied for this purpose is described in detail in Ref. [13]. The theoretical emission patterns were calculated by the “many beam” approach of electron motion in single crystals [11,15], using Doyle Turner potentials [16] in order to describe the electron-atom interaction. Due to the high atomic number of In, so-called “20-beam” simulations, in which the potential energy is approximated by 41×41 and the electron wave functions by 21×21 Fourier components, had to be used in order to obtain sufficient computational accuracy. We considered the following lattice sites: substitutional In (S_{In}) and P (S_{P}), tetrahedral interstitial T_{In} and T_{P} , anti-bonding AB_{In} and AB_{P} , bond center BC and hexagonal interstitial H (which are common to both sublattices), the so-called SP_{In} , SP_{P} , Y_{In} , Y_{P} , C_{In} , and C_{P} as well as various displacements from these positions along $\langle 111 \rangle$ and $\langle 100 \rangle$ directions. The location of these sites in the zinc blende structure is given in Ref. [17].

In order to extract correct lattice location information, the characteristic properties of the zinc blende structure have to be taken into account [14,17]. For instance, the $\langle 111 \rangle$ patterns do not allow one to discriminate S from T sites. In addition both the In and the P sublattice show the same projection along this direction. The best two-fraction fit to the $\langle 111 \rangle$ pattern [Fig. 1(e)] was obtained for 76% of emitter atoms on ($S+T$) sites with a root mean square (rms) displacement of $u_1=0.21$ Å and 24% on random (R) sites. Random sites are characterized by an isotropic emission yield, which can be due to emitter atoms occupying a variety of low-symmetric lattice sites or being located in disordered surroundings. Along $\langle 100 \rangle$ directions S_{In} and T_{P} sites lie within pure In rows while, e.g., S_{P} and T_{In} are located within pure P rows. Since the difference in the nuclear charge of In ($Z=31$) and P ($Z=7$) is quite pronounced, the $\langle 100 \rangle$ axis allows one to discriminate between ($S_{\text{In}}+T_{\text{P}}$) and ($S_{\text{P}}+T_{\text{In}}$) sites. The best three-fraction fit [Fig. 1(f)] was obtained for 85% on ($S_{\text{In}}+T_{\text{P}}$) with $u_1=0.22$ Å, 6% on ($S_{\text{P}}+T_{\text{In}}$) and 9% on R sites. Finally, the $\langle 110 \rangle$ and $\langle 211 \rangle$ patterns allow all various interstitial sites and both sublattices to be distinguished. Note that the sublattice sensitivity of the channeling patterns around the $\langle 110 \rangle$ and $\langle 211 \rangle$ directions is not only a consequence of the different nuclear charges along the In or P rows, but also a structural effect related to the lack of mirror-symmetry within the $\{110\}$ planes of the zinc blende lattice [14,17]. The best three-fraction fit for the $\langle 110 \rangle$ direction [Fig. 1(g)] was obtained for 76% of Er on S_{In} with $u_1=0.18$ Å, 6% on S_{P} and 18% on random sites. The best $\langle 211 \rangle$ fit [Fig. 1(h)] yielded 75% of Er on S_{In} with $u_1=0.15$ Å, 7% on S_{P} and 18% on random sites.

The angular width of electron channeling effects is approximately proportional to $Z^{1/2}$ while dechanneling lengths are roughly proportional to Z^2 [18], where Z is the mean nuclear charge along the atomic row from where the particle is emitted. The fact that Er occupies mainly substitutional In sites therefore has a characteristic influence on the channeling patterns along the $\langle 100 \rangle$, $\langle 211 \rangle$ and $\langle 110 \rangle$ directions. For emitter atoms on S_{In} sites, channeling along these directions is exclusively caused by In rows, and the angular width is large while at the same time dechanneling causes a considerable reduction of the maximum yield [15]. For comparison, the dechanneling lengths for the most tightly bound $1s$ -wave states of 200 keV electrons are 140 Å along $\langle 111 \rangle$, 79 Å along $\langle 100 \rangle$, 47 Å along $\langle 110 \rangle$ and 114 Å along $\langle 211 \rangle$ directions. Dechanneling is even responsible for the occurrence of a local yield minimum along the $\langle 100 \rangle$ axis [Figs. 1(b,f)]. Emitter atoms on substitutional P sites, on the other hand, should result in channeling effects with much narrower angular widths and higher maximum yields [Figs. 2(a-c)].

Excluding the S_P sites from the fit resulted in considerable degradation of the chi square of the fit, which became 12% worse for the $\langle 100 \rangle$, 11% worse for the $\langle 110 \rangle$ and 7% worse for the $\langle 211 \rangle$ patterns. The consistent increase in the chi square provides strong evidence that Er atoms occupy indeed some S_P sites. However, due to the rather small fraction of Er on these sites, it was not possible to determine the rms displacements from phosphorus sites reliably. While interstitial T_P and T_{In} sites produce the same $\langle 100 \rangle$ channeling patterns as S_{In} and S_P sites, respectively, the $\langle 110 \rangle$ and $\langle 211 \rangle$ patterns for these sites are distinctly different from both substitutional sites. To illustrate this we have shown the patterns due to T_P sites in Figs. 2(e-f). Fits including also Er on tetrahedral interstitial T_P or T_{In} sites resulted in minor improvements of the chi square values while the corresponding fractions on both positions were less than 4%, which is below the statistical uncertainty for such high-symmetric sites. Including additional lattice sites such as bond centered (BC), anti-bonding (AB), hexagonal (H) or various displaced sites also yielded only insignificant improvements in fit quality; possible fractions on these sites are estimated to be below 10%.

In conclusion, the most probable location of Er are 78(4)% on S_{In} sites with $u_1=0.19(3)$ Å, 6(3)% on S_P and 15(4)% on R sites. Note that the rms value of $u_1=0.19(3)$ Å could be due to an ensemble of Er atoms with small displacements from the In sites, but also to a fixed static displacement d of the order of $d = 3^{1/2} u_1 = 0.30$ Å. Comparison of the Er lattice location results in InP to Er in GaAs shows a striking difference. Whereas Er in GaAs is partly found on or near tetrahedral interstitial sites [19,20], most likely T_{As} sites [14], we could not identify such an interstitial fraction in InP.

Fig. 3 shows the results of an annealing sequence up to 550°C. Clear channeling effects were already visible directly following room temperature implantation, corresponding to 28% of Er on S_{In} and 3% on S_P sites. The remaining Er atoms occupy random sites, i.e. sites in disordered surroundings. The channeling effects improved markedly following annealing at 100°C and 150°C, resulting in the Er fractions on S_{In} and S_P sites discussed above. This annealing step is known from literature as the main structural recovery step for implantation damage in InP [15,21]. For annealing temperatures above 250°C in vacuum, the channeling effects decreased continuously. We attribute this to beginning thermal erosion of the near-surface layers since following annealing at 550°C all channeling effects completely disappeared along with a visible degradation of the sample surface.

Conclusions

Following the main structural annealing step of irradiation damage around 150°C, we have found the majority (~75%) of implanted Er in InP on substitutional In sites. The displacements from these sites were small, of the order of $u_1=0.19(3)$ Å in the case of isotropic displacements such as lattice vibrations, or around $d=0.30$ Å for static displacements. A second, much smaller fraction of Er (~7%) was found on substitutional P sites. Possible fractions on interstitial sites such as T_{In} or T_P were below the detection limit of a few per cent.

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Figures:

Fig. 1. (a)-(d): Channeling patterns from ^{167m}Er following room temperature implantation of ^{167}Tm into $n\text{-InP}$ and annealing at 150°C . (e)-(h): Best fits of simulated patterns to the experimental yields, corresponding to 76% of Er on S_{ln} and 7% on S_p sites.

Fig. 2. Theoretical $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 211 \rangle$ channeling patterns from 100% of $^{167\text{m}}\text{Er}$ on S_{P} (a-c) and T_{P} (d-f) sites.

Fig. 3. Fractions of $^{167\text{m}}\text{Er}$ on S_{In} , S_{P} and R sites as function of isochronal (10 min) annealing temperature.