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Lattice sites and damage annealing of Er in low-dose implanted GaAs

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Abstract

We have used conversion electron emission channeling to determine the lattice location of $^{167\text{m}}\text{Er}$ ($t_{1/2}=2.28$ s) in GaAs after 60 keV room temperature implantation of ^{167}Tm ($t_{1/2}=9.25$ d) at low doses ($0.6\text{--}3\times 10^{13}$ cm $^{-2}$). Following a recovery step of the implantation damage at 200-300°C, we observe a large fraction of Er (45-68%) on substitutional Ga sites. A second fraction of Er is found on the T_{As} sites (the tetrahedral interstitial sites with nearest As neighbours). The fraction on T_{As} sites reaches a maximum of 12-23% following annealing at 500-600°C. At higher annealing temperatures the channeling effects decrease markedly, which we attribute to the well-known degradation of GaAs due to As evaporation.

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Introduction

Erbium-doped semiconductors are of considerable interest as optoelectronic devices [1]. In general, the optical activity of Er is closely related to its lattice site and immediate surroundings. For Er in GaAs, theoretical investigations suggest that isolated Er prefers substitutional Ga sites (S_{Ga}) and that even the interaction with additional native defects such as Ga_i, As_i, or V_{As} is hardly able to remove it from this site [2]. Er on tetrahedral interstitial sites (T) is considered to be metastable, and the T_{As} sites should be lower in energy than the T_{Ga} sites.

On the experimental side, a number of Rutherford backscattering (RBS) lattice location studies on GaAs:Er revealed the following trends. In general, samples doped with Er during metalorganic chemical vapour deposition (MOCVD) [3-6] or molecular beam epitaxy (MBE) [7-9] showed the majority of Er in near-tetrahedral interstitial locations with respect to the GaAs lattice. A discrimination between T_{As} and T_{Ga} sites, however, was not considered in any of these studies. Er concentrations in these samples varied in a wide range from 10^{17} cm $^{-3}$ to 7×10^{20} cm $^{-3}$. The interstitial-like Er location in the high-dose regime was related to the formation of ErAs precipitates growing epitaxially along the GaAs <100> directions. In the low-dose doped samples, on the other hand, the interstitial position was ascribed to complexes between Er and carbon, which is a frequent contaminant in MOCVD. Samples which were intentionally co-doped with oxygen during MOCVD growth, however, showed mainly near-substitutional Er [6, 10].

Less studies have dealt with the lattice location of implanted Er in GaAs. Following high-dose implantation at 250°C (10^{15} cm $^{-2}$ at 150 keV, peak concentration of 2.8×10^{20} cm $^{-3}$) and annealing up to 1000°C, Er atoms were found within the <100> but partly outside the <110> atomic rows [11, 12]. While such a behaviour could be due to a mixture of substitutional (S) and tetrahedral interstitial (T) Er, it would also be expected for Er within large <100> epitaxial ErAs precipitates. Only the outermost Er atoms in the precipitates sense the particle flux-peaking within the <110> channel, at the same time they shadow the Er atoms in deeper ErAs layers [10]. Recently the Er sites following implantations at lower doses ($0.75\text{--}7.5\times 10^{14}$ cm $^{-2}$, 100-250 keV, $\approx 10^{19}\text{--}10^{20}$ cm $^{-3}$) and annealing at 850°C were investigated [13]. A 7.5×10^{13} cm $^{-2}$ implantation resulted in 80% of Er on S, 5% on T and 15% on random sites, while higher doses yielded only 10% on S, but 55% on T and 35% on random sites. In this work the interstitial fraction was ascribed to small ErAs precipitates.

In order to extend the Er lattice location studies to even lower doses, we have applied conversion electron emission channeling [14] from the short-lived isotope $^{167\text{m}}\text{Er}$ ($t_{1/2}=2.28$ s). This excited nuclear state is

populated as a consequence of the radioactive decay of the isotope ^{167}Tm (9.25 d) and deexcites 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 emission yield from the crystal surface which depends in a characteristic way on the lattice sites occupied by the emitter atoms. Previously we have already used this method to study the lattice sites of Er in Si [15, 16].

Experimental

The samples used in our experiments were two $\langle 100 \rangle$ cut n-GaAs:Te single crystals ($0.6\text{-}2 \times 10^{-3} \Omega\text{cm}$, $n=1\text{-}5 \times 10^{18} \text{ cm}^{-3}$). 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 doses of $6 \times 10^{12} \text{ cm}^{-2}$ (sample A) and $3 \times 10^{13} \text{ cm}^{-2}$ (sample B). These parameters correspond to [Tm+Er] peak concentrations of $3 \times 10^{18} \text{ cm}^{-3}$ (A) and $1.5 \times 10^{19} \text{ cm}^{-3}$ (B) at a depth of 198 Å (FWHM 78 Å). Following the room temperature implantations the samples were annealed capless in vacuum $< 10^{-5}$ mbar. In order to detect the angular-dependent emission yield of the 150, 199 and 206 keV conversion electrons emitted by ^{167}mEr we used the position- and energy sensitive detection system described in Ref. [16].

Results and discussion

Fig. 1(a)-(c) show the normalized ^{167}mEr conversion electron emission yields around the $\langle 111 \rangle$, $\langle 100 \rangle$ and $\langle 110 \rangle$ directions of sample A following the annealing sequence to 300°C . Pronounced emission channeling effects are visible along all axial and planar directions, which is clear evidence that the majority of ^{167}mEr occupies 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 procedures applied for that purpose are described in detail in Ref. [16]. The theoretical emission patterns were calculated using the "many beam" approach of electron motion in single crystals [14].

Extracting reliable lattice location information for the III-V compound GaAs requires to consider the characteristic properties of the underlying zincblende structure [17]. For instance, the $\langle 111 \rangle$ patterns do not allow to discriminate between S and T sites; in addition both the Ga and the As sublattice show the same projection along this direction. The best fit to the $\langle 111 \rangle$ pattern [Fig. 1(d)] was obtained for 85% of emitter atoms on (S+T) sites with a root mean square (rms) displacement of $u_1=0.2 \text{ Å}$ and 15% on random (R) sites. Along $\langle 100 \rangle$ directions S_{Ga} and T_{As} sites lie within pure Ga rows while S_{As} and T_{Ga} are located within pure As rows. By T_{As} we denote those T sites which have 4 nearest As neighbours in $\langle 111 \rangle$ and 6 next-nearest Ga neighbours in $\langle 100 \rangle$ directions. In principle the $\langle 100 \rangle$ axis could therefore allow to discriminate between ($S_{\text{Ga}}+T_{\text{As}}$) and ($S_{\text{As}}+T_{\text{Ga}}$). However, the nuclear charges of Ga and As are so similar that in practice it is impossible to distinguish the $\langle 100 \rangle$ Ga and As rows reliably. The best fit [Fig. 1(e)] was obtained for 82% on (S+T) with $u_1=0.16 \text{ Å}$, and 18% on R sites. Finally, the $\langle 110 \rangle$ patterns allow to distinguish between all various interstitial sites and between both sublattices. Rather than being a consequence of the different nuclear charges of the $\langle 110 \rangle$ Ga or As rows, the sublattice sensitivity is a structural effect related to the mirror-asymmetry of the $\langle 110 \rangle$ directions of the GaAs lattice. Hence Er preferring sites in one specific sublattice, e.g., S_{Ga} , causes an asymmetry in the $\langle 110 \rangle$ patterns. On the other hand, if the Er would be equally distributed among both sublattices, the electron yield around the $\langle 110 \rangle$ direction should be almost symmetric with respect to mirroring at the $\{100\}$ plane, which is not the case [Fig. 1(c)]. Best fits [Fig. 1(f)] were obtained for 65% of Er on S_{Ga} with $u_1=0.16 \text{ Å}$, 16% on T_{As} , and 19% on random sites. Excluding the T_{As} sites from the fit resulted in a 15% worse chi square. Due to the rather small fraction of Er on T_{As} , it was not possible to determine the rms displacement from this site reliably. Fits including also Er on S_{As} or T_{Ga} resulted in a few percent improvement of the chi square values while the corresponding fractions on both sites were less than 5%, which is about the statistical uncertainty. Including additional lattice sites such as bond centered (BC), anti-bonding (AB), hexagonal (H) or displaced sites also yielded only insignificant improvements in fit quality; possible fractions on these sites are estimated to be below 10%.

Fig. 2 summarizes the results of the annealing sequences for both samples. In both cases clear channeling effects were already visible directly following room temperature implantation, corresponding to around 38% of Er on S_{Ga} sites in the low-dose sample A, and 13% in the higher-dose sample B. The remaining Er fraction occupies random sites, i.e. sites in disordered surroundings which are responsible for an isotropic electron emission yield. In sample A the channeling effects improved markedly following annealing at 200°C , resulting more or less in the Er fractions on S_{Ga} and T_{As} sites discussed above. On the other hand, in sample B the recovery step was shifted to higher temperatures and a larger amount of Er (50%) remained on R sites. This behaviour indicates incomplete structural recovery of the radiation damage in this higher-dose implanted sample.

In between the annealing steps at 600°C and 650°C, sample A was heated again at 500°C for 2 h in order to measure *in situ* the emission channeling effects at this temperature. The results were essentially the same as measuring at room temperature following the 600°C anneal (Fig.2). This shows that the S_{Ga} sites are thermally stable during the life time of the excited ^{167m}Er state and not only metastable positions which are populated as a consequence of the ^{167}Tm decay.

In both samples a smaller part of Er was found on the T_{As} sites. In sample A the fraction on T_{As} grew with increasing annealing temperature up to 500°C on the expense of the S_{Ga} sites. Upon annealing to 650°C, the T_{As} fraction decreased to zero, while the substitutional S_{Ga} fraction was still around 35%. In sample B, on the other hand, less Er was found on T_{As} sites, and the maximum occurred after annealing around 625°C, when the fraction on S_{Ga} sites had already considerably decreased. Er on T_{As} sites can not be explained by the formation of epitaxial ErAs precipitates, since the Er atoms at the surface of the precipitates are supposed to be located on T_{Ga} sites [13]. Moreover, we would also expect that the probability of forming such clusters and hence the fraction of Er on T-like sites would be higher in the higher dose sample B. The increasing occupation of T_{As} sites is therefore not well understood at the moment. The vanishing of the channeling effects following annealing above 600°C is not astonishing. It has been reported in the literature that vacuum annealing of GaAs above 500°C without As overpressure or capping causes excessive As losses within the first few hundred Å and sample degradation [18].

Conclusions

We have extended the earlier results of Alves et al [13], who found the majority of implanted Er in GaAs on substitutional sites, to even lower doses. Moreover, we give direct evidence that, in agreement with theoretical predictions [2], Er prefers the S_{Ga} sites. The displacements from these sites were found to be small, of the order of $u_1=0.16-0.20$ Å in the case of isotropic displacements such as lattice vibrations, or around $d=0.20-0.25$ Å for static displacements. A second, smaller fraction of Er was found on T_{As} sites, also in agreement with predictions that the T_{As} sites should be the most stable interstitial sites for Er. However, more detailed experiments will be required to better understand the thermal behaviour of the fractions of Er on both S_{Ga} and T_{As} sites.

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Figures

Fig. 1. (a)-(c): Channeling patterns from ^{167m}Er following room temperature implantation of ^{167}Tm into n-GaAs:Te and annealing at 100°C, 200°C and 300°C for 10 min. (d)-(f): Best fits of simulated patterns to the experimental yields, corresponding to the Er fractions on S_{Ga} and T_{As} sites given in the text.

Fig. 2. Fractions of ^{167m}Er on S_{Ga} , T_{As} and R sites as function of isochronal (10 min) annealing temperature for samples A (a) and B (b). All measurements were done at room temperature, except the open data points for sample A, which were measured at 500°C following the 600°C anneal.