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EXAFS study of the structural properties of In and In + C implanted Ge

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Abstract. The structural configurations of In implanted Ge have been studied via x-ray absorption spectroscopy with and without the codoping of C. In the case of In singly implanted Ge, while the In atoms occupy an substitutional site in Ge ($InGe_4$) at low In concentration (≤ 0.2 at. %), they precipitate into a metallic phase (In metal) and form complexes composed of one vacancy and three Ge atoms ($InVGe_3$) at concentration ≥ 0.6 at. %. This behaviour can be suppressed by the addition of C leading to In-C pairing to form $InCGe_3$ complexes. This cluster enables In atoms to recover a four-fold coordinated structure and has the potential to improve the electrical activation of In atoms in Ge.

1. Introduction

It is widely accepted that an alternative channel material replacing Si is required to maintain CMOS (complementary metal-oxide semiconductor) performance improvements with a scaling beyond the 14-nm technology generation [1]. Ge has been considered as a promising candidate as it offers superior electron (~ 2×) and hole (~ 4×) mobilites compared to Si [2]. The low activation energy (0.012 eV) and low diffusion coefficient of In in Ge makes it an ideal *p*-type dopant, which benefits both device performance and scaling [3]. Since the lattice structure significantly influences the electrical properties, a detailed study of the In-doped Ge atomic configuration is necessary to understand the effects of doping concentration and defect environments that ensue with processing.

Recent lattice site location studies employing the emission channeling technique concluded that at low In implantation fluences (2.9×10^{12} In atoms/cm^2), In preferentially occupies Ge bond-centered sites before annealing and then redistributes to substitutional lattice sites after 300 °C annealing [4]. In-vacancy (In_mV_n) clusters within the Ge lattice were found to be energetically favourable by density functional theory (DFT) calculations [5]. In the case of In + C co-implanted Ge, substitutional In-C pairs in the Ge lattice were detected by perturbed angular correlation (PAC), and C co-doping was thus considered to be an approach to improve the electrical properties by compensating the strain caused by oversized In atoms in the Ge lattice [6]. Complementary atomic information such as coordination numbers (CN), nearest neighbour (NN) type and bond length are still undetermined for In-rich Ge and In + C co-implanted Ge, a knowledge of which could potentially enable correlation of the atomic environment to the electrical properties as a function of In concentration.

In this work, we employed extended x-ray absorption spectroscopy (EXAFS) to characterize the atomic environment of In-doped Ge as a function of In concentration and C co-doping, examining the configurations of the In absorber with Ge, V and C.

2. Experimental Methods

In ions were implanted into undoped 1.8 µm (100)-Ge on Si substrates at 250 °C with In concentrations ranging from 0.02 to 1.2 at. %. C was co-implanted before the In in selected samples to the same concentrations. The In concentrations for the two sample sets were measured by Rutherford backscattering spectrometry. A three step annealing process was applied, at temperatures of 550, 450 and 350 °C for 0.5, 1, 2 h, respectively, in N_2, to initially activate In dopants and reduce lattice disorder. Fluorescence mode XAS measurements were performed at the XAS beamline of the Australian Synchrotron at the In *K* edge, with a Si (3 1 1) double crystal monochromator and a 10 × 10 pixel-array Ge solid state detector [7]. Data analysis was carried out using the IFEFFIT package based on the FEFF9 code [8]. To aid the simulations and fits of the EXAFS spectra, four different models were proposed as in Figure 2, after structural optimizations within DFT calculations performed with the VASP code [9].

3. Results and Discussion

Figure 1(a) shows the Fourier transformed (FT) EXAFS spectra of the In-doped Ge samples. It is clear that the 0.02, 0.06 and 0.2 at. % samples share a similar spectrum, while the 0.6 and 1.2 at. % samples are comparable to the In standard. The fits of the data confirm this argument. For samples with In concentration ≤ 0.2 at. %, In atoms occupy a substitutional site in a highly ordered Ge matrix, consistent with model (a) in Figure 2 and in agreement with the results from emission channeling [4].

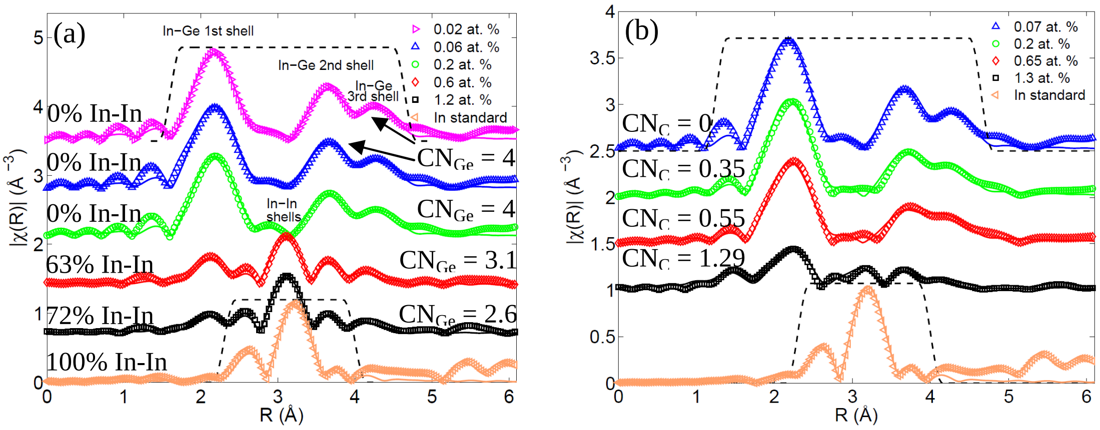

Figure 1. The magnitude of Fourier transform of k^2 weighted EXAFS spectra in radial distance (*R*-range), markers represent the data points while the solid lines are the best fits, where (a) is the result for In implanted Ge samples and (b) for In + C implanted Ge samples (Ref. [10]). The In metal fraction and coordination number of Ge in the first shell (in (a)), and the coordination number of C in the first shell (in (b)) are indicated above the spectrum. Reprinted with permission from J. Appl. Phys. **118**, 165701 (2015). Copyright 2015, AIP Publishing LLC.

For the 0.6 and 1.2 at. % samples, the FT EXAFS spectra appear to be comprised of substitutional In and metallic In. However, a combination of models (a) and (b) in Figure 2, where substitutional In atoms have a first shell of four Ge atoms, yielded non-physical Debye-Waller factors (DWFs) in the EXAFS analysis. As a consequence, model (c) in Figure 2 was invoked after a structural relaxation using a DFT calculation, where the Ge coordination number for In atoms in the non-metallic environment was allowed to vary with $CN_{Ge} \leq 4$. The resultant fit qualities were much improved using a combination of models (b) and (c), attesting to the validity of this approach. The fits of 0.6 and 1.2 at. % samples yielded 63 % metal fraction with CN_{Ge} = 3.1 and 72 % metal fraction with CN_{Ge} = 2.6, respectively. The precipitation of In was confirmed by transmission electron microscopy (TEM) and

XANES analysis [10], and the $InVGe_3$ cluster configuration used here was supported by the earlier DFT studies [5]. A more comprehensive investigation about these samples was provided in our previous work [10].

In our earlier report, the In metal precipitation and In-V clusters were found to be electrically inactive in Ge as expected [10]. Aiming to suppress the formation of these electrically inactive structures and enhance the In atom active fraction at high concentration, C was introduced as a co-dopant.

For an In concentration of 0.07 at. %, the EXAFS spectra (Figure 1(b)) are comparable with and without C co-implantation. The high quality fit of the co-implanted sample with model (a) confirmed that the In atoms are in substitutional sites of Ge without In-C pairing. The low concentrations of both In and C yields a low probability of In-C pair formation.

In-C pairs were found in the 0.2 at. % co-implanted sample. Though it has an EXAFS spectrum similar to that without C (Figure 1) and the first scattering peak in the FT spectra shows In atoms are substitutional, the smearing of the second and third peaks implies more disorder in the In surroundings. Indeed, model (a) was not able to provide a good fit for the second and third peaks. A model of a substitutional In atom coordinated with a C atom (model (d)) was thus proposed. After a DFT geometry optimization, the relaxed model shows that the introduction of a nearest neighbour C atom separates the second and third Ge atom shells into six different shells (with distances of 3.51, 4.10, 4.38, 4.45, 4.82 and 5.09 Å). The paired C component was allowed to vary given not all In atoms are expected to form pairs. An improved quality fit was obtained using model (d). The number of NN C atoms was 0.35 for the 0.2 at. % In+C implanted Ge sample. In-C pair formation starts before the In precipitation concentration is reached.

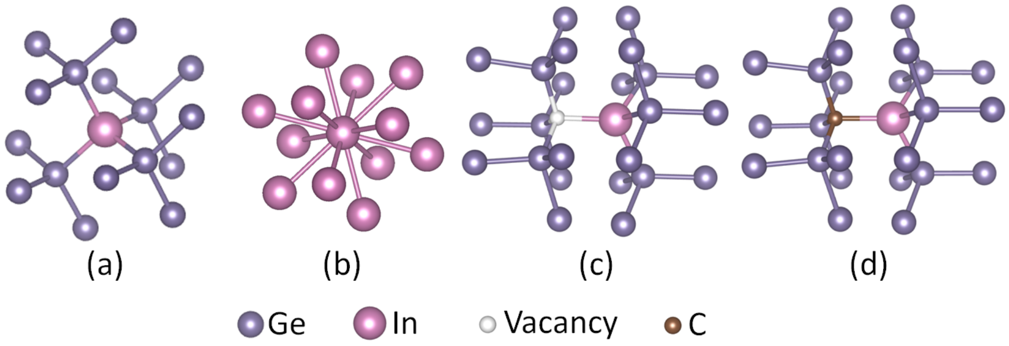

Figure 2. Schematics of models of (a) In atom in the substitutional site of Ge lattice ($InGe_4$), (b) In metal, (c) In atom coordinating with a vacancy in the substitutional sites of Ge lattice ($InVGe_3$) and (d) In atom coordinating with a C atom in the substitutional sites of Ge lattice ($InCGe_3$)

For In and C concentrations $\geq$ 0.65 at. %, Figure 1(b) shows that the amplitude of the In metal peaks were dramatically reduced for co-implanted samples with the spectra more similar to that of substitutional In than metallic In. The In metallic precipitation at high doping concentration was obviously suppressed when C was co-implanted as supported by TEM and XANES analysis (not shown). The reduction of In metal precipitation is a consequence of the formation of substitutional In–C pair ($InCGe_3$ cluster) in the Ge lattice. For the 0.65 at. % In+C doped sample, a considerable smearing of the second and third peaks is visible in the EXAFS spectrum, which is an indication of In-C pair as described above. The fit of the spectrum using model (d) gave the NN C atoms coordination number to In of 0.55.

For the 1.3 at. % sample, a good fit was also obtained using the same approach, with the number of NN C atoms being 1.29. The peak at ~3 Å in FT spectrum of the 1.3 at. % sample was due to the Ge atoms in the 3.51 Å shell, which was not observed in the 0.2 and 0.7 at. % samples due to their low fraction of In–C pairs. A low spectral amplitude was visible, which means the In atoms are in a highly disordered environment. In fact, the Ge lattice was polycrystalline as observed by TEM due to the high implanted concentration of both In and C atoms.

The bond lengths calculated from the fits of the EXAFS spectra were in good agreement with those from the DFT calculation for both In and In + C implanted samples. Alternative models were tested in the fits of the EXAFS spectra, but yielded low fitting quality or non-physical DWFs. A binding energy of -0.46 eV was calculated for an In-C pair in Ge by Chroneos *et al*. [11] using DFT, indicating that pairing is energetically favourable as experimentally demonstrated here. Our results were also supported by the PAC measurements of Tessema *et al*. [6] who observed In-C pairing when the annealing temperature was below 650 °C. Not only the In metal precipitation was suppressed by co-doping C, evidence of In-V cluster was also not found in the In+C co-implanted Ge samples according to the XAS analysis. With the introduction of C, an improvement of In atom activation was achieved with the apparent reduction of both electrical inactive In complexes and In atoms recover into a four-fold coordinated structure ($InCGe_3$).

4. Conclusion

In conclusion, the structural properties of In implanted and In+C co-implanted Ge have been analysed by XAS. When In was singly implanted in Ge, the In atoms precipitate from the substitutional sites of Ge and form In metal and In-V clusters when the In concentration is ≥ 0.6 at. %. The formation of these two electrical inactive In related clusters was successfully suppressed by co-implanting C, which leads to In-C pairs occupying substitutional sites of Ge. The reduction of electrically inactive complex formation and the recovery of In atoms back to the four-fold coordinated structure enhanced the In atom activation in Ge.

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