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THE STRUCTURAL ENVIRONMENT OF Te DOPANTS IN GaAs USING EXAFS IN FLUORESCENCE MODE

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Abstract

The local co-ordination of 'grown-in' Te in GaAs has been determined by FLEXAFS measurements. At carrier concentrations of $8 \times 10^{18}$ cm$^{-3}$ considerable dilation of the first co-ordination sphere around the dopant takes place, with appreciable contraction of the second co-ordination sphere. The first, second and third nearest neighbour distances were found to be 2.58 ($\pm 0.02$) Å, 3.52 ($\pm 0.05$) Å and 4.58 ($\pm 0.1$) Å, respectively. These are discussed in terms of various models which have been proposed for group VI dopants in GaAs.

Introduction

The structural and electronic effects of dopant impurities in tetrahedral semiconductors can, in general, be predicted according to a simple mis-fit model as described by Vegard's Law. However, in the case of GaAs there are a number of dopants (e.g. Sn, Te, Se) which dilate the lattice to a much greater extent. Te doping has received specific attention and several studies have shown that this dilation is considerable at concentrations of greater than $10^{18}$ cm$^{-3}$ [1]. It has thus provided a useful model system for studying dopant environments in III-V semiconductors.

Experiment and Analysis

Single crystal wafers of GaAs were obtained which were about 2.5 cm in diameter and contained 'grown-in' impurity concentrations of Te, the measurements reported here relate to a carrier concentration of $8 \times 10^{18}$ cm$^{-3}$. Reflection X-ray topographs revealed the wafer to be of good crystal perfection, with no large-scale mosaicity. FLEXAFS spectra were recorded at the Te K-edge using the Wiggler station 9.2 on the SRS at SERC Daresbury Laboratory. The wafer samples were inclined at an angle of approximately 10 degrees to the incident monochromatic beam, and rotated in their plane to average out any Laue diffraction effects in the recorded spectrum.

Several scans were averaged to achieve adequate signal/noise. To assist in data analysis standard spectra were also recorded. These were measured in transmission mode using powdered samples of GaAs (for the Ga and As K-edges) and elemental Te (for the Te K-edge). Fig. 1 shows the $k^3$ weighted spectra for As and Ga in GaAs, together with the phase-shift corrected Fourier transforms. Three shells of the zinc-blende structure can be readily identified and the equivalence of the As and Ga sites is well reproduced. The EXAFS of Te and its atomic distribution are shown in...
fig. 2; elemental Te has a chain structure and the intra and inter chain correlations can be clearly seen. Data sets were background subtracted, Fourier transformed and least-squares refined with the aid of the Daresbury EXCURVE program [2]. The dotted curves in fig. 2 show the fit to experiment using the curved wave theory [3]. They have been omitted from fig. 1 for clarity but the distances, FWHM widths and co-ordination numbers for As and Ga are included in Table 1. Fig. 3 shows the weighted EXAFS spectrum and Fourier transforms for Te impurities in GaAs. The dotted line is the least-squares fit to experiment and the structural parameters for the first three shells are also included in Table 1.

Fig. 1. $k^3$ weighted Ga (---) and As (----) K-edge EXAFS and Fourier transforms for GaAs.

Fig. 2. $k^3$ weighted K-edge EXAFS and Fourier transforms of elemental Te. The dotted lines are the 'curved wave' theory fits.

Fig. 3 demonstrates that the dopant environment of Te is quite distinct from the matrix environment of As and Ga. Note that the first shell is dilated and the second shell is contracted for Te compared to As (or Ga). In particular the first shell radius of 2.58 Å is 0.13 Å longer than the As-Ga bond length, indicating considerable relaxation to accommodate the larger anion. The second shell radius of 3.52 Å is 0.47 Å shorter than the equivalent shell in the zinc-blende structure, indicating the possibility of a vacancy in this shell. The third shell also appears to be slightly contracted, although this change is outside the precision of analysis.
Fig. 3. $k^3$ weighted Te K-edge EXAFS and Fourier transform of $8 \times 10^{18}$ cm$^{-3}$ Te doped GaAs. Dotted lines give 'curved wave' theory fits. Parameters are included in Table 1.

Table 1. Interatomic distances, shell widths and co-ordination numbers from the analysis of spectra shown in figs. 1 to 3.

<table>
<thead>
<tr>
<th>Shell</th>
<th>Distance (Å)</th>
<th>FWHM (Å)</th>
<th>Co-ordination Number</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pure Doped</td>
<td>Pure Doped</td>
<td>Pure Doped</td>
</tr>
<tr>
<td>1</td>
<td>2.45 2.58</td>
<td>0.17 0.15</td>
<td>4 4</td>
</tr>
<tr>
<td>2</td>
<td>3.99 3.52</td>
<td>0.28 0.18</td>
<td>12 11</td>
</tr>
<tr>
<td>3</td>
<td>4.65 4.58</td>
<td>0.29 0.22</td>
<td>12 12</td>
</tr>
</tbody>
</table>

Models

(a) Te in the As site with Ga vacancies in the first shell. This is a fairly common model for the Te incorporation and has been proposed by Huang [4] and Mullin et al. [5] (amongst others). This would be expected to reduce the first shell co-ordination number and introduce some disorder. This is not observed.

(b) Te on an As site with Ga interstitials in the first shell. This was proposed by Mullin et al. [5] and could certainly explain the dilation observed. However, it would also lead to an increase in the first shell co-ordination number.

(c) A Te/Ga interstitial complex aligned along [100] positioned on a Ga site and associated with a Ga vacancy. Such a defect was proposed by Fewster [6]. This defect would split the first co-ordination shell and provide some shorter Te-Ga and Te-As contacts, which are clearly not seen (fig. 3).

(d) Te on an As site associated with As vacancies in the second shell. This has not yet been suggested for Te but a recent structural study by Sette et al. [7] has proposed such a model for S-doped GaAs at a level of between $2 \times 10^{19}$ and $2 \times 10^{20}$ atoms cm$^{-3}$. In the case of Te in GaAs with this model we would expect a large expansion of the first shell, together with a relaxation of the second shell. The second shell co-ordination number should also be reduced.
Conclusions

Model (d) provides the closest agreement with the environment of Te we have measured (see Table 1). Unlike the case of S, where the first shell disorder was found to be greater than the second or third shells, pointing to a mixture of sites, we find the widths of all three shells are as narrow (or slightly narrower) than for Ga or As and conclude that Te EXAFS at a carrier concentration of $8 \times 10^{18}$ cm$^{-3}$ relates to a single substitutional site.

Acknowledgements

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References