On the site occupancy of dopants in 4H-SiC

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Silicon carbide (SiC) is a semiconductor material which is widely used for devices operating under extreme conditions. The fabrication of planar electronic devices requires a high concentration of p- and n- dopants. This can be archieved preferentally by ion implantation because of the small diffusion coefficients of dopants in SiC. After implantation, the implan-ted atoms predominantly occupy interstitial lattice sites [1], where they are usually not electrically active. Therefore, a thermal postimplantation annealing process is necessary to electrically activate the implanted dopants and to reduce the lattice damage, however, for the case of high foreign atom concentration, the SiC matrix remains defective always [2]. Another possibility to avoid lattice defects is to incorporate the doping element in-situ during the epitaxial growth of the crystal which can be performed by chemical vapour deposition (CVD) Concerning the site occupancy of p and n dopants a number of questions remains [3,4] from Hall mobility measurements.

In this paper this question will be addressed using a combined analysis of convergent beam electron diffraction (CBED) and ALCHEMI (atomic location by channelling enhanced microanalysis) for the case of Al implanted 4H-SiC. The shift of Higher Order Laue Zone (HOLZ) lines appearing in CBED patterns can be used for detection of very small lattice parameter changes ([5,6,7]). However from this shift the origin of the strain can not be distinguished e.g. whether the foreign atoms occupy lattice or interstitial sites. By means of ALCHEMI the site occupancy of atoms within a matrix lattice can be determined [8]. This method has been applied for the case of Ge implanted in SiC already [9].

Aluminium implanted hexagonal 4H-SiC (concentrations: $5*10^{19}$ cm^{-3} for ion implantation at 160keV and $7*10^{17}$ cm^{-3} - $2*10^{20}$ cm^{-3} for CVD implanation) have been investigated using CTEM, CBED and ALCHEMI. CBED patterns were obtained on [120 80 1] at an operating high voltage of 300kV. The EDX analysis was made on [01-10] zone axis incidence for tilts of ±1/2g to ±5/2g with g=0004.

CBED patterns revealed different changes in HOLZ line shapes for different dopant concentrations, which can be attributed to different lattice distortion. Models of lattice distortion were suggested and calculated by Molecular Dynamics. Their influence on the HOLZ lines appearance was simulated by the multislice method. To determine the positions of the implanted atoms inside the unit cell, the CBED simulations have been carried out for probable locations of dopants in the SiC lattice (on lattice sites, on interstitials sites or both lattice and interstitial sites) by using the results of the ALCHEMI experiments.

The comparison of ALCHEMI simulations and experiments (Fig. 1 and 2) showed that in the CVD growth case the implanted Al is mostly substituting Si in the matrix and in the ion-implanted sample Al is occupying Si-lattice positions and interstitials in equal parts. The CBED experiments (Fig. 3) show a line split of a line (1-1-22) in the CBED pattern in the ion-implanted samples and no split of that line in the CVD growth samples which can be understood from the substitution of Si by Al.

1. S. Virdis, U. Vetter, C. Ronning, H. Kröger, H. Hofsäss, J. Appl. Phys. 91-3 (2002) 1046
2. U. Kaiser, D.A. Muller, J.L. Grazul, A. Chuvilin, M. Kawasaki, Nature Materials 1 (2002), 102
3. D.J. Larkin et al. Appl. Phys. Lett. 65 (13) (1994), 1659
4. W.J. Choyke NATO ASI Series E: Appl. Scien. Vol 185 (1999), 853
5. J.M. Zuo, M. Kim, R. Holmestead, J. Electron. Microsc. 47 (1998), 121

6. U. Kaiser, K. Saitoh, K. Tsuda, M. Tanaka, J. Electron. Microsc. 48 (1999) 221
7. S. Krämer, J. Mayer, C. Witt, A. Weickenmeier, M. Rühle, Ultramicroscopy 81 (2000) 245
8. J.C.H. Spence, J. Tafto, J. of Microscopy 130 (1983) 147
9. U. Kaiser, J. Electron Microscopy 50 (2001) 251
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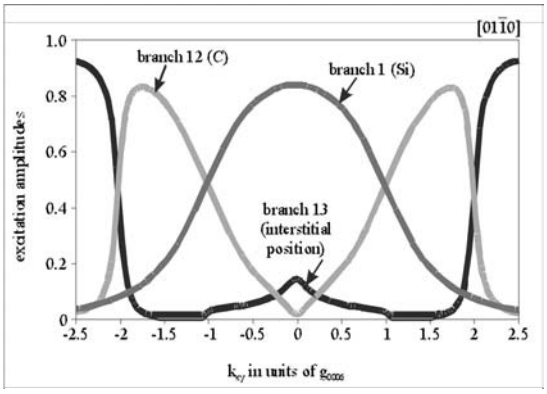

Figure 1. Calculated exitation amplitudes for [01-10] zone axis and three possible lattice sites (Si-, C- and intersitial position). Because the of different curves for the three positions the determination of the location of dopants is possible.

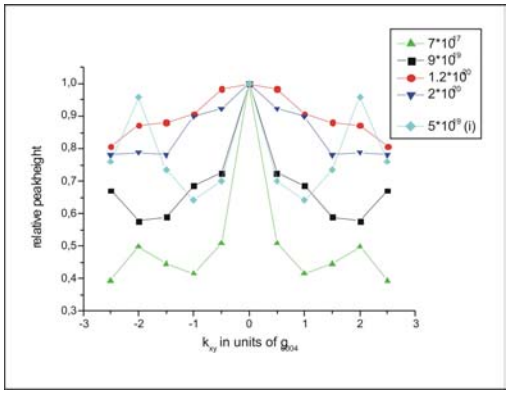

Figure 2. Experimental results: relative x-ray Al-peak heights for different tilt conditions. The index (i) marks the ion-implanted sample. The relative measurement error is below 10%. Comparison with Figure 1: The Al is mainly occupying Si-Position for ▲,■,●,▼ samples and interstitials (♦).

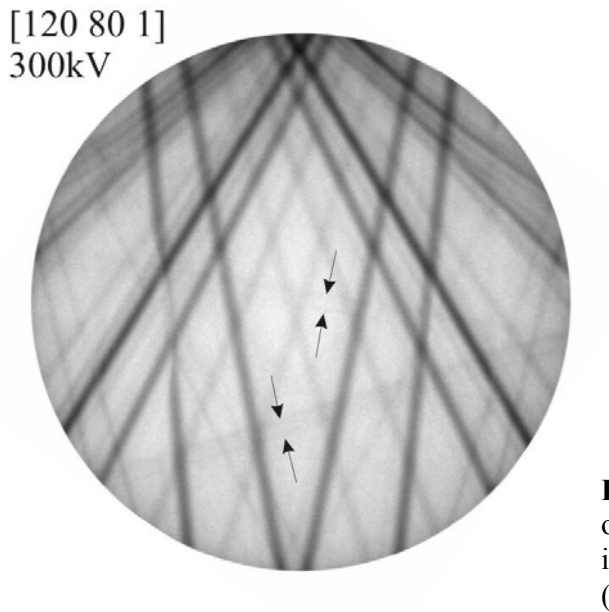

Figure 3. Experimental CBED pattern of [120 80 1] of Al doped 4H-SiC (ion-implantation). Splitting of (1 –1 –22) nd (1 –2 19) lines is marked by arrows.