Ab-initio study of the effects of defects on the electronic mobility in 4H-SiC

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Introduction

Among the many polytypes of silicon carbide, 4H-SiC has the highest carrier mobility with the least anisotropy, combined with a large band gap of 3.2 eV. Along with this, its low leakage current and high breakdown voltage make it a good candidate for high-temperature electronics. In addition, its high radiation hardness makes SiC a potential candidate material for radiation detectors in extreme conditions with respect to temperature and irradiation.

At elevated temperature, SiC is less susceptible to defect formation. However, at low temperatures, where self-annealing is weak, point defects such as vacancies, interstitials, and their clusters do not only provide traps for the charge carriers, but also act as scattering centers and thus affect their mobility.

In order to understand the resulting mobility degradation and predict the reduced device life and performance, previous work has fitted a total effective change in the mobility as a function of irradiation dose to experimental measurements [1-2]. This however does not help to understand which defects are the dominating species, and how effective each of them is as a scattering center. Following Restrepo et al. [3], we perform self-consistent Density Functional Theory (DFT) calculations to model the effect of various defects on the electronic mobility in 4H-SiC.

$$\mu_{\alpha\beta} = -\frac{2e}{n_c}\sum_n \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\tau_n(\mathbf{k})\,\mathrm{v}_\alpha(\mathrm{n}\mathbf{k})\mathrm{v}_\beta(\mathrm{n}\mathbf{k})\frac{\partial \mathrm{f}(\mathrm{E}(\mathrm{n}\mathbf{k}))}{\partial \mathrm{E}} \quad (1)$$

Method and simulation:

The mobility is calculated from the Boltzman transport equation with a relaxation time calculated from the scattering potential of a particular defect. The scattering probabilities for the relaxation time are determined with the help of Fermi's Golden Rule. Using Matthiessen's rule, the overall effect of various defects on the mobility can then be calculated. We use the Vienna Ab-initio Simulation Package (VASP) and Quantum Espresso for the first principles calculations, and the defect scattering potentials are determined from supercells with 128 atoms.

Results and Discussion:

Figure 1 shows the calculated scattering potential due to an N-dopant at a C-site. Figure 2 shows the effect of various defects on the electronic mobility, for an assumed concentration of $1x10^{16}$ cm^{-3} at room temperature. Combining these results with SRIM simulations for 5 MeV α-particles with a dose of 10^{13} cm^{-2}, we find that the mobility reduces to 32 cm^2/V-s just after irradiation.

Interstitials degrade the mobility by the largest extent, while antisites have the smallest effect. While interstitials are energetically less favorable than antisites and, should have a negligible concentration in 4H-SiC at thermal equilibrium [4], continuous irradiation in operation can create significantly non-equilibrium conditions with high interstitial concentration, especially at low temperature and, reduce carrier mobility. At sufficiently high temperatures, the interstitials would recombine or transform into antisites, minimizing the radiation effect on the carrier mobility.

Conclusions:

Using parameter free DFT self consistent calculations, the effect of various defects on the electronic mobility in 4H-SiC has been studied. It has been observed that interstitials are most harmful to the electronic mobility.

Acknowledgements:

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References:

1. R. P. Joshi, *Monte-Carlo calculation of temperature & field dependent electron transport parameters in 4H-SiC,* J. Appl. Phys. **78**, 5518 (1995)
2. J. Pernot, S. Contreras, J. Camassel, J. L. Robert, W. Zawadzki, E. Neyret, L. Di. Cioccio, *Free electro density and mobility in 4H-SiC,* Appl. Phys. Lett. **77**, 4359 (2000).
3. O. D. Restrepo, K. Varga, S. T. Pantelides, *First principles calculations of electronic mobilities in silicon: phonon and coulomb scattering*, Appl. Phys. Lett. **94**, 212103 (2009).
4. F. Gao, M. Posselt, V. Belko, Y. Zhang, W. J. Weber, *Structure and energetics of defects: a comparative study of 3C and 4H-SiC*, Nucl. Instr. and Methods in Phys. Res. B **218**, 74 (2004).

Figures

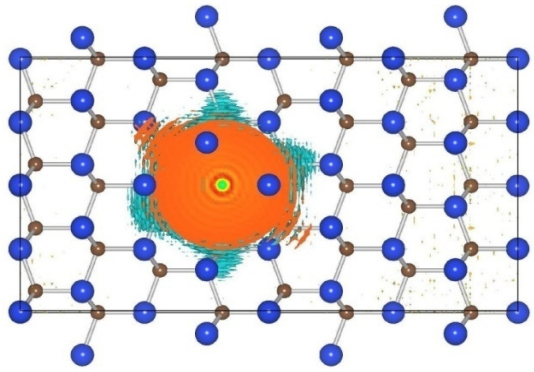

Figure 1: Ab-initio calculated scattering potential for a N-impurity substituting a C-atom in 4H-SiC. Large blue spheres respresent Si atoms, small brown spheres C atoms.

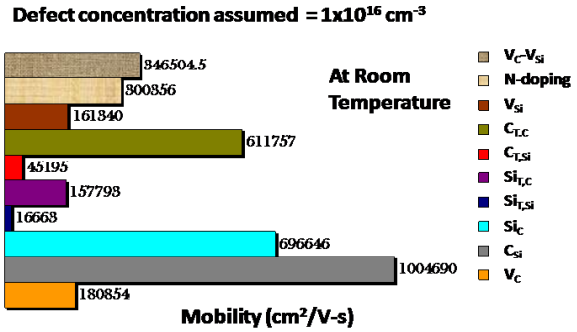

Figure 2: Effect of various defects on the electronic mobility in 4H-SiC, calculated at room temperature for an assumed concentration of $1x10^{16}$ cm^{-3}. A tetrahedral Si interstitial in a tetrahedron between Si atoms affects the mobility most adversely, while a C_{Si} antisite, where a C atom replaces a Si atom, shows the smallest effect. $A_{T,X}$ denotes an A atom in a tetrahedral interstitial site surrounded by X atoms.