Eva Rauls, *Annealing Mechanisms of Point Defects in SiC – A Theoretical Investigation*
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Abstract

Due to the high computational demands of first principle methods and the low accuracy of (semi-)empirical methods, only little is known about the dynamics of defects in semiconductors. However, an understanding of these matters is crucial for technological progress in e. g. device fabrication. In this work, an approximate method with an accuracy comparable to that of first principle methods has been chosen to investigate migration mechanisms of intrinsic point defects like vacancies and antisites, as well as of common n-type dopants, in silicon carbide (SiC). The selfconsistent charge density-functional based tight-binding (SCC-DFTB) method allows a systematic investigation of defect dynamics, which to this extent is virtually impossible to first principle methods.

The formation of antisite aggregates has been investigated, starting with a discussion of several mechanisms for the creation of the antisite pair $C_{Si}\,Si_C$, which is a promising candidate for the origin of the D_I-photoluminescence. Calculated activation energies show that vacancy migration plays a key role in the mobility of antisites and, thus, in aggregate formation. Although larger aggregates of antisites have been found to be extremely stable, their creation seems only to be possible by a special epitaxial method during growth. Since energy barriers are lower for recombination with an assisting vacancy than for antisite pair creation, two-dimensional aggregation stops after the creation of one antisite pair. For the formation of "onion-like" structures like $Si_C\,(C_{Si})_4$ a mechanism based on the mobility of C_{Si} has been found. Including the usually neglected entropical contributions to the energy does not change the results qualitatively, although it is shown that these contributions are not negligible at temperatures as high as required for the activation of the discussed processes.

It has recently been reported that the free charge carrier concentration saturates at high concentrations during n-type doping of SiC with nitrogen. In order to understand this observation, we have studied the annealing behavior of implanted nitrogen ions in SiC. Carbon split-interstitials $(CC)_C$ can mobilize substitutionally built in nitrogen by creating nitrogen split-interstitials $(NC)_C$. Calculations based on the migration of these split-interstitials have confirmed that nitrogen prefers to be built in on the carbon site. In contrast to carbon vacancies, silicon vacancies are not simply filled up by the N-atoms, but instead the $(NC)_C$ undergoes a kick-out mechanism which leads to either $V_{Si}\,N_C$ or $C_{Si}\,N_C$ pairs. The $V_{Si}\,N_C$ pair is the first step to the formation of the very stable $V_{Si}(N_C)_4$ complexes, which have been calculated to be electrically inactive, so that we can explain the observed high passivation of dopants. For phosphorus, as an alternative n-type dopant, an even more efficient split-interstitial based migration mechanism has been found. Investigations on recombination processes of phosphorus split-interstitials $(PC)_C$ and $(PSi)_{Si}$ with vacancies show that phosphorus can be built in on both silicon and carbon sites, in contrast to nitrogen. The formation of inactive complexes as found for nitrogen is hindered thereby, making P the preferred n-type dopant over N.

Keywords

Silicon Carbide (SiC), Density-Functional Theory, Tight-Binding, Point Defects, Aggregation, Diffusion, Annealing, Ion Implantation