

Investigation of Unintentional Impurity-Related Defect Aggregation Within Bulk 4H-SiC

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To create p-doped regions within 4H-SiC MOSFET devices, 4H-SiC is bombarded with high energy Al⁺ ions from gaseous AlH₃ during ion implantation. However, recent experimental studies have found channel mobility-affecting shallow electron and hole donor states whose densities are directly proportional to Al implantation concentration [1-4]. Despite test structures of these studies having undergone post oxidation anneal in NO atmospheres, which is renowned for reducing 99% of interfacial state densities [5], these defects are found with densities in the range of 4×10^{11} - 4×10^{14} cm⁻² [2,3]. Use of high Al concentrations during implantation has been linked to the precipitation of Al clusters [6] via identification of impurity band conduction [7] within, alongside secondary ion mass spectrometry (SIMS) imaging [8] of, heavily Al-doped 4H-SiC layers. As well, Low-Energy Muon-Spin-Rotation Spectroscopy (LE- μ SR) measurements have also indicated that unintentional doping can occur in SiC during NO anneal, with N-carrier concentration increases of almost two magnitudes being observed [9]. If unintentional N-doping occurs during NO anneal, then unintentionally co-doping would also be taking place in p-doped devices, with different separately introduced p- and n-type impurity related defects aggregating together to create defect complexes with shallower ionization energies than the original dopant impurity [10]. Subsequently, there is a likelihood that NO-passivation interactions during post oxidation anneal are taking place with precipitated clusters of Al atoms at the device interface, to form defect complexes involving Al-N and Al-O.

We investigate the possibility of Al-O and Al-N complex formation within SiC devices, as well as whether such complexes can be correlated with the experimentally found mobility reducing states, using density functional theory (DFT) calculations. For each complex, four different geometry configurations corresponding to impurity substitution at different hexagonal (HEX) and cubic (CUB) lattice sites, derived using the Site-Occupancy Disorder package [11], were studied. Incorporation and binding energies, and charge transition levels (CTL) of these complexes were calculated in bulk 4H-SiC with the PBE0 functional.

For all 8 configurations, only the neutral (0) and first negative (-) charge states are found to be stable in the 4H-SiC bandgap. Within the 4H-SiC bandgap, the formation energies of these two charge states are negative for all configurations, signalling that formation of these complexes is more favourable than Al, N, and O atoms remaining within a gaseous atmosphere of AlH₃ and NO. Specific configurational geometry is likely not a limiting factor in formation of these complexes as well. Also, negative binding energies were obtained for all configurations, indicating that, if Al_{Si} and N_C/O_C are separately present within 4H-SiC, it is more energetically favourable for them to form aggregates. For both complexes, the same geometry configuration is found to have the lowest formation and binding energies, the shallowest $-/0$ CTLs, and the most delocalised bandgap defect state. The 'band-like'-ness of these defect states is believed to be a major contributor towards the configurational favourability. The $-/0$ CTLs of 3 Al-N geometry configurations and the lowest energy Al-O configuration are found to coincide with the activation ranges of the experimentally found channel mobility-affecting shallow electron and hole donor states.

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