The Pan African Conference on Crystallography (PCCR2)
and
The African Light Source Conference (AfLS2)

Contribution ID: **85** Type: **Poster Presentations**

Induced defect levels of P and Al vacancy-complexes in 4H-SiC: A hybrid functional study

Tuesday, 29 January 2019 17:15 (5 minutes)

The electronic behaviour of high-dose phosphorus implanted in 4H-SiC is mainly desirable to obtained lower sheet resistance of 4H-SiC. Al doping on the other hand acts as an acceptor, improves the dielectric properties of 4H-SiC and has very low diffusivity in SiC. Using a hybrid density functional theory, we investigated the properties of Al and P defect-complexes in 4H-SiC a wide band-gap semiconductor that is promising for applications in high-frequency and high-temperature electronic device. We show that vacancy-complexes formed by P_{Si} and Al_{Si} are more energetically stable than those formed by P_C and Al_C. The defects with silicon vacancy are predicted to experience more lattice distortion compared to those formed with carbon vacancy. While vacancy-complexes formed with P_{Si} or P_C and V_C induced double donor levels, vacancy-complex formed with substitution of P and V_{Si} induced negative-U charge state ordering. The Al with V_C related vacancy-complexes induced deep single donor and acceptor levels, and Al with V_{Si} induced only acceptor and negative-U ordering.

Summary

We have used DFT from first-principles to predict the properties of various P and Al related vacancy-complexes in 4H-SiC: reporting their formation energies, binding energies, charge state transition levels and negative-U charge state ordering properties. The vacancy-complexes with silicon vacancy were predicted to experience more lattice distortion compared to those formed with carbon vacancy. The P and Al related vacancy-complexes showed that they are stable with respect to their binding energies under equilibrium conditions. While the vacancy-complexes formed by the P Si and Al Si are more energetically stable, the vacancy-complexes formed by P_C and Al_C had high formation energies. The P_{Si}V_C and Al_{Si} V_C are energetically most favourable defects at any Fermi-level in the band gap of 4H-SiC for P and Al related vacancy-complexes, respectively. This result also corroborate earlier report on the characterization of this defect. The defect levels induced by the P related vacancy-complexes are very shallow close to the conduction band minimum for the single and double acceptor levels, and deep for both the single and double donor levels. Furthermore, only the P_{Si} V_{Si} and P_C V_{Si} induced negative-U charge state ordering that are lying deep in the band gap of 4H-SiC. While the Al with V_C related vacancy-complexes on the other hand induced deep single donor and acceptor levels, the Al with V_{Si} induced only acceptor and negative-U charge state ordering. These results provide an insight for future work which is crucial for improving the quality of n-type SiC.

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Session Classification: AfLS2 Poster Session

Track Classification: AfLS2 track