

In this study, the properties of a number of defects commonly occurring in Czochrolaski-grown silicon and their reactions with each other and interstitial hydrogen were investigated. The calculations were performed using density functional theory with the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional. For each defect, its charge-state transition levels were determined and, where possible, compared to other theoretical results as well as to experimental values.

The calculated results for the carbon-oxygen related defects showed that, at zero charge state, both the complexes and the hydrogen passivated complexes are stable. The donor and acceptor levels predicted for the C_i , O_iH_i , $C_sC_iH_i$ C_sC_i , and $C_iO_iH_i$ agree with deep level transient spectroscopy (DLTS) measurements to an acceptable level of accuracy, and hydrogen passivation shifted the donor and acceptor levels out of the band gap. In the case of the C_iO_i , and C_iH_i defect complexes, one charge state showed a good agreement with experiment while the other was not observed experimentally. However, in the case of the $C_sO_iH_i$ defect complex, there is inconsistency between the experiment and one theoretically predicted level while the other level agreed well with the experiment.

For the $C_iO_i(Si_i)_n$ defect complexes in the neutral charge states the binding energies confirmed the stability of the C_iO_i , $C_iO_iSi_i$ and the $C_iO_i(Si_i)_n$ defect complexes as well as the ability of H_i to bind to the complexes. Binding with H_i moved the donor levels into the conduction band and the acceptor levels into the conduction band. The predicted defect levels showed good agreement with the available experimental and previous theoretical results.

The calculated binding energies suggested that O_i , C_s , Bi , B_s , and O_{2i} may react to form stable defect complexes of BiC_s , BiO_i , B_sBi , B_sO_i , B_sO_{2i} and BiO_{2i} defect complexes in the neutral charge state. As previously, the results also predicted that H_i can bind to the defect complexes. The theoretically predicted levels agree very well with the reported experimental values, and the negative-U properties of the Bi were also correctly predicted. Except for the B_sBi defect complex, hydrogen passivation shifted the donor levels into the conduction band while the acceptor levels were shifted into the valence band. In contrast, the B_sBi defect complex is electrically inactive but after hydrogen passivation, a donor level at $E_v + 0.50$ eV was predicted.

The theoretical predictions of the binding energies suggest that V_2 , VO_i , V_2O_i , VO_{2i} , D_sVO_i , $D_sV_2O_i$, and D_sVO_{2i} (where D may be Pb , Ge or Sn) are stable defect complexes in their neutral charge state. The predicted charge state transition levels indicated that all the defect complexes are electrically active with defect levels that agree reasonably well with the experimental and previous theoretical results. Hydrogen passivation shifted the defect levels of V and V_2 defect complexes towards the valence band for the donor levels and towards the conduction band for the acceptor levels. Whereas, for the rest of the defect complexes, hydrogen passivation brought the defect levels to the mid of the band gap which would probably make the defects very efficient recombination centres. Isovalent doping by Ge , Sn or Pb caused the defect levels to become shallow and hydrogen passivation only slightly shifted the donor levels to the valence band and the acceptor levels to the conduction band.