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Identifying radiation induced point defect in SiC nanowires: computational modeling. MING UU, University of Louisville — SiC nanowires (NWs) are expected to possess higher radiation tolerance compared to their crystalline counterpart due to their efficiency in eliminating point defects generated by the radiations. In this study, we will develop a computational modeling scheme to identify the radiation induced point defects in SiC NWs. A preliminary study on the hexagonal 2H-SiC NWs has demonstrated that the point defects on the surface of the SiC NWs only create local distortions and will not cause the destruction of the entire structure of the SiC NWs. It is also found that the local strain created by the antisite, the C-vacancy, and the Si-interstitial defects induces a few impurity states inside the energy gap, while defects such as the Si-vacancy and C-interstitial defects tend to produce a small tail at the top of the valence band. These observations suggest that the electronic properties of the SiC NWs will not be affected to any great extent by these types of points defects on the surface of the SiC NWs, and therefore the SiC NWs are expected to be tolerant or resistant responding to these types of radiation effect.

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