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Modelling Radiation Induced Vacancy-Interstitial Clusters

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High energy particle irradiation created cluster defect model is based on the particle bombardment process scenario. The incident particle strikes the crystal lattice at the point of interaction and initiate the movement of lattice ions along with itself. The moving group of ions leave the vacancy region behind itself and further destroy the lattice structure causing other ions to leave their stable crystalline positions. By the end of destruction process the three defect regions are formed: region of vacancies, disordered region of randomly distorted lattice ions and the region of interstitials. These three subregions form the vacancy-interstitial defect cluster. After the irradiation the relaxation of defect region may take place with interstitials returning back to the vacancy positions thus partially restoring crystalline lattice structure within a defect cluster.
The electronic states within such a cluster and its environment are calculated using density functional method. Compared to earlier simulation results obtained by E. Holmström et al (2010) and our group (E. Zasinas et al, 2014, 24th Cern RD50 workshop) the newly proposed cluster defect model has a much richier deep level structure. The earlier studied cluster model was considered as a region of randomly displaced ions giving rise to acceptor type of deep level states originating from the broken interatomic valency bonds. The model presented in this work exhibit both acceptor states and donor states. It is suggested that the broken valency bonds in vacancy subregion give rise to the deep level acceptor states and the valency electrons of the extra atoms in the interstitial atoms subregion give rise to the deep level donor states. Thus sush an assymetric deffect cluster may act both as acceptor and donor type of deffect in electronic devices.
E. Holmström et al, Phys. Rev. B 82, 104111 (2010).

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