Contribution ID: **5** Type: **not specified**

Modelling Vacancy-Interstitial Clusters and their effect on on Carrier Transport in Silicon

Wednesday 11 June 2014 11:00 (20 minutes)

High energy particle bombarding creates both point defects and clusters of defects within the target material. We model such a cluster of defects in silicon crystal as a few nanometer size region of randomly displaced ions which may be understood also as an aggregate of vacancy and interstitial defects. The electronic states within the cluster and its environment are calculated using density functional method. The results of calculations performed on 25 randomly created clusters exhibit the presence of deep level states within the silicon band gap. These localized states originate mainly from the broken interatomic valency bonds. Further structure relaxation of cluster modelled by the same density functional theory calculations and in practice realized as annealing lead either to restoration of ordered crystal structure or to formation of more energetically stable cluster of vacancy and interstitial defects. In the last case the great part of broken bonds are reconnected and the number of deep level states is diminished. The remaining deep level states act as acceptors of the conduction band electrons. After being charged by the captured electrons these acceptors highly concentrated within the cluster create an electrostatic potential substantial enough to modify the transport of charge carriers. This in turn leads to modification of voltamperic characteristics of silicon semiconductor structures and devices.
To model the macroscopic effect of cluster defects introduced into semiconductor device we use the Synopsys TCAD software tools. We show that the defect clusters modify conduction properties of silicon sample. The electrostatic potential barriers created by randomly distributed clusters prevent the free carrier movement and the conductivity of the sample is greatly reduced. However if the electric field of the applied external voltage is stronger than the one of these microscopic potentials the defect clusters have no effect and the conductivity of the sample is restored.

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Session Classification: Session 1 - Defect and Material Characterization