Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A2]Symposium A-2

Chair: Kenjiro Sugio(Hiroshima Univ., Japan)

Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6

[SY-A2]From first-principles defect chemistry to device damage models of radiation effects in III-V semiconductors

○Peter A Schultz, Harold P Hjalmarson (Sandia National Laboratories, United States of America)

An atoms-to-circuits assessment of radiation damage in microelectronics begins with understanding atomic displacement damage in a semiconductor material, the subsequent evolution of the radiation-induced defect populations in the material, and propagating this understanding into defect-aware damage models for continuum-scale device simulations. The foundation of a multiscale modeling framework to understand long-time, device-scale response is a quantitative description of the dominant atomic processes using quantum mechanical modeling. We describe the development of a comprehensive radiation-induced defect reaction network in Si-doped (n-type) and C-doped (p-type) GaAs using density functional theory (DFT), identifying mobile species and consequent defect reactions, characterizing defect properties needed to formulate the chemistry needed in defect physics models for device simulations. In turn, the device simulations solve a set of drift-diffusion equations to evolve a model chemistry, and predict the electrical response of device of a specified configuration and operating conditions. The upscaling bridge from the atomistic description given by DFT and experimental defect spectroscopies to a device description of radiation response proves to have many challenges. We describe the successes and also the remaining outstanding challenges in standing up a full first-principles motivated hierarchical multiscale model of radiation damage in electronic devices. ---
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