Migration Processes of the As Interstitial in GaAs and InGaAs

A. F. Wright, N. A. Modine, S. R. Lee and S. M. Foiles

Sandia National Laboratories, Albuquerque, NM 87185, USA

Thermal and carrier-induced migration processes of the As interstitial in GaAs have been studied using density-functional theory (DFT) and the local-density approximation (LDA) for exchange and correlation. The most important thermal processes were found to involve the -1, 0 and +1 charge states and to produce migration along <110>-type directions. In the -1 and 0 charge states, migration proceeds via hops between stable *split-interstitial* configurations at bulk As sites through saddle-point configurations in which the As interstitial *bridges* two adjacent bulk As sites. In the +1 charge state, the roles of these two configurations are approximately reversed and migration proceeds via hops between stable bridging configurations through metastable split-interstitial configurations, which are bounded by slightly distorted split-interstitial configurations. Calculated activation energies for thermal migration in the 0 and +1 charge states are in good agreement with measured activation energies in semi-insulating and *p*-type GaAs. Also consistent with observations, the approximate reversal of the stable-state and saddle-point configurations in the 0 and +1 charge states is found to enable carrier-induced migration via a Bourgoin-Corbett mechanism with a residual activation energy of 0.05 eV.

As interstitial migration via these same thermal and carrier-induced processes has also been studied in an $In_{0.5}Ga_{0.5}As$ alloy. In this case, kinetic Monte Carlo (kMC) simulations are required because the stable-state and saddle-point energies of the As interstitial depend on its nearby group-III site occupations and, hence, on its location in the alloy. To enable these simulations, we developed parameterized models (*cluster expansions*) of the As interstitial stable-state and saddle-point energies in the alloy based on DFT results for *training sets* of alloy configurations having different nearby group-III site occupations. Results from the kMC simulations display qualitatively and consequentially different migration from what is found in GaAs.

This work was supported, in part, by Sandia's Solid-State Lighting Science Energy Frontier Research Center, sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.