Migration Processes of the As Interstitial in GaAs and InGaAs

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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.

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