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Atomistic simulations in nanostructures composed of tens of millions of atoms MAREK KORKUSINSKI, GERHARD KLIMECK, HAIYING XU, SEBASTIEN GOASGUEN, FAISAL SAIED, Purdue University, West Lafayette, IN 47906 USA, SEUNGWON LEE, Jet Propulsion Laboratory, California Institute of Technology — Strain in self-assembled quantum dots (QDs) is a long-range phenomenon, and its realistic determination requires a large computational domain. To find it for a dome-shaped InAs QD with diameter of 19.2 nm, the nanoelectronic modeling tool NEMO-3D uses the atomistic VFF Keating model with domain sizes of up to 64 million atoms. Interatomic distance changes thus obtained are used to influence the sp3d5s* tight-binding electronic Hamiltonian defined on a subdomain containing up to 21 million atoms (matrix size of order of $4x10^8$). Targeted eigenstates with correct symmetry are found reliably even in such large systems. NEMO-3D is used to analyze the dependence of the QD states on the size of the strain domain and the boundary conditions. The energies of a deeply embedded QD depend dramatically on the strain domain size. For QDs buried under a thin capping layer, on the other hand, the existence of a free surface at the top of the sample allows for an effective relaxation of atoms, and the penetration of strain into the barrier is small.

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