Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Atomistic calculation of electronic and optical properties of a single InAs quantum dots M. ZIELINSKI, M. KORKUSINSKI, Institute for Microstructural Sciences, NRC, Ottawa, Canada, W. SHENG, Department of Physics, Fudan University, Shanghai, China, P. HAWRYLAK, Institute for Microstructural Sciences, NRC, Ottawa, Canada — We present an atomistic tight-binding (TB) theory of electronic structure and optical properties of a single self-assembled InAs quantum dot (SAD). In previous work an effective-bond-orbital model (EBOM) was used to calculate electron and hole states of the SAD. The strain distribution was calculated using the continuum elasticity theory and EBOM was coupled to the strain via the Bir-Pikus Hamiltonian. However, the properties of these multimillion-atom systems are influenced by the presence of crystal facets and the symmetry of underlying zinc-blende lattice. In current work we present a fully atomistic TB model, accounting for the atomistic symmetry, and extended to include d-orbitals for proper treatment of interband/intervalley couplings. Strain is included in the Hamiltonian via Slater-Koster rules and a generalized Harrison law, with the equilibrium positions of atoms calculated using the valence force field method. Coulomb matrix elements are found using the TB functions, and electronic properties of N confined excitons (N=1-6) are determined in the CI approach. Emission spectra of multiexcitons are also obtained. Comparison with the previous approach and the experimental results is presented.

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Date submitted: 26 Nov 2007 Electronic form version 1.4