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Atomic-Scale Modeling of Shape Stability-Regimes and Stacking in InAs/GaAs Quantum Dot Nanostructures THOMAS HAMMERSCHMIDT, PETER KRATZER, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — From a thermodynamic point of view, quantum dot (QD) growth is governed by the balance between energy gain due to strain relief and energy cost due to formation of QD side facets and edges. Both contributions are accounted for by an interatomic potential of the Abell-Tersoff type that we developed recently. We relax realistic InAs/GaAs QD nanostructures using this interatomic potential and compare the resulting total energies. To investigate the experimentally observed shape sequence of 'hut'-like QD's dominated by {317} facets and 'dome'-like QD's dominated by {101} facets, we compare the energy of a homogenous InAs film and differently sized InAs QD's with either shapes. We identify three regimes: For coverages below about 1.9 monolayers InAs the film is most stable, followed by small 'hut'-like QD's and larger 'dome'-like QD's. This is in line with the experimentally deduced critical coverage for the 2D to 3D growth transition, and the shapes of small and larger QD's. We can also explain the growth correlation in QD stacks: Our calculated potential-energy surfaces of free-standing QD's in different lateral positions above overgrown QD's show an energy gain of about 20 meV per In atom for the experimentally observed vertical QD alignment.

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