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An Investigation into InAs/GaAs Thin Film Growth[1] MARIA MIGNOGNA, KRISTEN FICHTHORN, Penn State University — Quantum dots self-assemble due to Stranski-Krastinov growth in heteroepitaxial systems with a lattice mismatch above 2%, for example in the deposition of InAs on GaAs (001). However, there are many questions left unanswered about quantum dot growth, such as the role of strain in the wetting layer. Simulation techniques such as molecular dynamics (MD) can provide insight at the atomic scale. An empirical potential to study this system has recently been developed [1]. Using NPT MD, we studied the thermal properties and melting of bulk GaAs, as well as the stability of the GaAs(001)β2(2x4) reconstruction against melting. To probe diffusion and the preferred Ga-atom binding sites, we calculated the minimum potential-energy surface for a gallium atom on the GaAs (001) β2(2x4) reconstruction. We also evaluated various diffusion pathways and energy barriers using the nudged elastic-band method. The potential captures the location and energy of the deepest binding minimum as compared to DFT values and also achieves good agreement for the diffusion barriers. We used accelerated MD simulations to obtain diffusion coefficients as a function of temperature and these compare favorably to previous results from experiment and DFT. [1] T. Hammerschmidt, PhD Thesis (2006)

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