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Multi-scale simulation of quantum dot formation in Al/Al (110) homoepitaxy[1] YOGESH TIWARY, KRISTEN FICHTHORN, Penn State University — In experimental studies of Al(110) homoepitaxy, it is observed that over a certain temperature window (330-500K), 3D huts, up to 50 nm high with well defined and smooth (111) and (100) facets, form and self-organize over the micron scale [1]. The factors leading to this kinetic self-organization are currently unclear. To understand how these structures form and evolve, we simulated multi-layer, homoepitaxial growth on Al(110) using ab initio kinetic Monte Carlo (KMC). At the high temperatures, where nano-huts form, the KMC simulations are slow. To tackle this problem, we use a technique developed by Devita & Sander [2], in which isolated adatoms make multiple moves in one step. We achieve high efficiency with this algorithm and we explore very high temperatures on large simulation lattices. We uncover a variety of interesting morphologies (Ripples, mounds, smooth surface, huts) that depend on the growth temperature. By varying the barriers for various rate processes, we discern the factors that determine hut sizes, aspect ratios, and self-organization. [1] F. Buatier de Mongeot, W. Zhu, A. Molle, R. Buzio, C. Boragno, U. Valbusa, E. Wang, and Z. Zhang, Phys. Rev. Lett. 91, 016102 (2003). [2] J.P. Devita & L.M. Sander, Phys. Rev. B 72, 205421 (2005).

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