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Controlling Self-Assembly in Al(110) Homoepitaxy YOGESH TIWARY, KRISTEN FICHTHORN, Pennsylvania State University — Homoepitaxial growth on Al(110) exhibits nanoscale self-assembly into huts with well-defined (100) and (111) facets [1]. Although some of the diffusion mechanisms underlying this kinetic self-assembly were identified and incorporated into a two-dimensional model [2], we used density-functional theory (DFT) to identify many other mechanisms that are needed to describe the three-dimensional assembly seen experimentally [3]. We developed a three-dimensional kinetic Monte Carlo (KMC) model of Al(110) homoepitaxy. The inputs to the model were obtained from DFT [3,4]. Our model is in agreement with experimentally observed trends for this system. We used KMC to predict self-assembly under various growth conditions. To achieve precise placement of Al nanohuts, we simulated thermal-field-directed assembly [5]. Our results indicate that this technique can be used to create uniform arrays of nanostructures. [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] W. Zhu, F. Buatier de Mongeot, U. Valbusa, E. G. Wang, and Z. Y. Zhang, Phys. Rev. Lett. 92, 106102 (2004). [3] Y. Tiwary and K. A. Fichthorn, submitted to Phys. Rev. B. [4] Y. Tiwary and K. A. Fichthorn, Phys. Rev. B 78, 205418 (2008). [5] C. Zhang and R. Kalyanaraman, Appl. Phys. Lett. 83, 4827 (2003).

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