Abstract Submitted
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An Accelerated Molecular Dynamics Study of the GaAs (001) β2(2x4) Reconstruction[1] MARIA MIGNOGNA, KRISTEN FICHTHORN, Penn State University — The GaAs (001) β2(2x4) reconstruction is the most commonly used substrate for growth in GaAs homoepitaxy by molecular beam epitaxy. While the atomic positions of the β2(2x4) unit cell have been determined, reflection high energy electron diffraction and scanning tunneling microscopy images show long range disorder on this surface[1]. It is hypothesized that domains of anti-phase β2(2x4) unit cells can be created by vacancies or As dimer shifts. Accelerated molecular dynamics (MD) allows us to examine atomic scale processes that can lead to this disorder. We have developed an adaptive accelerated MD scheme based on the bond boost method of Miron and Fichthorn[2]. The adaptive method is suitable for the rough energy landscape presented by GaAs (001). In the adaptive method, both the length thresholds for determining transition states and the magnitude of the boost are calculated on the fly. We are able to extend the physical timescale of the simulation by several orders of magnitude. We see events that lead to small domains of As dimers shifting. By simulating RHEED images of the surface, we link the disorder to experiment. [1] D.W. Pashley, J.H. Neave, B.A. Joyce, Surf. Sci., **582**, 189 (2005) [2] R.A Miron, K.A. Fichthorn, J. Chem. Phys., **119**, 6210 (2003)

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