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Accelerated Molecular Dynamics of GaAs(001) Homoepitaxy: Effects of Long-Range Disorder[1] YANGZHENG LIN, KRISTEN FICHTHORN, Penn State University — GaAs homoepitaxy and heteroepitaxy are both fundamentally and technologically significant. From a fundamental perspective, recent experimental work has shown that the GaAs(001) β2(2x4) substrate can transform and play an active role in diffusion and the morphologies that form during thin-film growth. Structural transformations lead to a substrate with local (2x4) domains that exhibit long-range disorder characteristic of c(2x8). At experimentally relevant temperatures, these transformations are mediated by rare events that occur over time scales ranging from ns to ms, which makes it difficult to probe the kinetics with conventional rare-event techniques. We develop an accelerated molecular dynamics (MD) protocol to deal with this challenge and we apply it to describe the temperature-dependent long-range structure of the surface. Our results are in agreement with experiment. Adatom diffusion occurs over longer time scales than those associated with transformations of the surface. Our accelerated MD studies indicate that adatom diffusion on this surface occurs via different mechanisms than those suggested by previous theoretical studies based on first-principles density-functional theory.

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