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**On the Genesis of Ge/Si Epitaxial Interfaces: Tracking the Behavior of Deposited Atoms Using Molecular Dynamics with Analytic Bond Order Potentials**

Kurt SCHEERSCHMIDT<sup>1#</sup>, Oussama MOUTANABBIR<sup>2</sup>

<sup>1</sup>Max Planck Institute of Microstructure Physics, Germany, <sup>2</sup>Department of Engineering Physics, Polytechnic School of Montreal, Canada

<sup>#</sup>Corresponding author: [schee@mpi-halle.de](mailto:schee@mpi-halle.de) <sup>+</sup>Presenter

Surface phenomena play a crucial role in defining the nature and quality of heteroepitaxial interfaces [T. Leontiou, et al., Phys. Rev. Lett. 105 (2010) 236104] and nanostructures [O. Moutanabbir et al., Phys. Rev. Lett. 105 (2010) 026101]. Inarguably, developing an atomistic understanding of these phenomena is one of the key challenges towards controlling the epitaxial growth of thin films and nanoscale structures. In this perspective, molecular dynamics (MD) simulations have been performed to study the atomic processes involved in early stage of deposition of Ge atoms on a Si surface. Our simulations employ a bond order potential extended to order 4, which is based on the tight binding (TB) model [K. Scheerschmidt, V. Kuhlmann, Int. J. Mat. Res. 98 (2007) 11-21 and Phys. Rev. B 75 (2007) 014306.]. It preserves the essential quantum mechanical nature of atomic bonding and achieves O(N) scaling by diagonalising the TB-Hamiltonian recursively, which enables fast and accurate MD simulations on macroscopic time and length scales beyond the realm of ab initio calculations. After relaxation of initial models, e.g., SiGe islands on Si surfaces at a few hundreds K, additional Ge are deposited with varying energy and momentum about every some 10000 integration steps of 1fs. Varying MD and deposition conditions unravelled an ensemble of processes governing the early stage of heteroepitaxy including surface diffusion, the mixing and exchange of atoms as well as the assembly of two-dimensional islands. Tracking these processes provides unique insights into the behavior of deposited atoms throughout the early stage of heteroepitaxy. Our simulations will be discussed in the light of recent experimental studies of morphological and elemental properties of Ge evaporation on Si using solid-source molecular beam epitaxy.