GPU-accelerated computational modeling of Moiré-regulated metal nanocluster self-assembly on 2D bilayer surfaces

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Abstract

Bilayer graphene with a top layer rotated with respect to a bottom one typically forms a periodically corrugated surface called a Moiré superlattice. This surface presents a complex potential energy landscape for diffusion of deposited atoms or molecules, which can be exploited to assemble nanoclusters with well-defined positions and sizes. We numerically constructed Moiré superlattices and corresponding potentials for various values of a twist angle and strain, and followed with a formulation of a nonlinear diffusion equation for continuous submonolayer adsorbate coverage field $\rho\left(x, y, t\right)$, accounting for adsorbate-adsorbate interatomic interactions via the Sutton-Chen potential. Then we analytically determined a quasi-2D steady-state nanocluster distributions by solving a model reduced to one spatial dimension. We next computed solutions of a full, 2D nonlinear diffusion problem for Pt, Ni, and Pb adsorbates in three temperature regimes and determined the kinetics of approaching a steady-state distributions. As the alternative and complimentary approach, we formulated a Langevin equation for diffusion of individual atoms on a Moiré and computed the extensive statistics of diffusion for various random initial configurations of atoms. We also determined stable final nanocluster configurations of N atoms using these computations and a graph-theoretical approach.

Biography of Presenter

Prof. Mikhail Khenner has the PhD degree from the Université Aix-Marseille II, France and Perm State University, Russia. He did postdoctoral studies in Tel Aviv University and University of Delaware. He is with the Department of Mathematics at WKU since 2009. He is the author and co-author of over fifty publications on modeling crystal growth, thin films, pattern formation and self-assembly. He was invited speaker at various national and international conferences in materials science and mathematical modeling. He routinely collaborates on research projects with physicists, applied mathematicians, materials scientists, and engineers. He co-authored two textbooks and is a reviewer for top-ranked professional journals.