

Investigating the Mechanisms of Remote Epitaxy: Interfaces, Interactions, Nucleation, and Defects

S.W. Schmucker¹⁺, M.X. De Jesus Lopez^{1,2}, S. Addamane¹, Q. T. Campbell¹, P. Lu¹, A. Rice¹, K.S. Jones², J.C. Koepke¹⁺

¹ Sandia National Labs, 1515 Eubank Blvd SE, Albuquerque, NM 87123

² University of Florida, 549 Gale Lemerand Dr., Gainesville, FL

Remote Epitaxy refers to epitaxial growth on a crystalline substrate coated with a two-dimensional (2D) material. In this process, the epi-layer is oriented to, but not covalently bonded with, the substrate, which facilitates detachment and hetero-integration. This configuration also allows for dynamic rearrangement or “sliding” relaxation at the 2D interface, thereby reducing defects in the epi-layer.

Our results indicate that for the growth of AlN films on SiC substrates, a greater fraction of relaxed AlN is achieved when grown on graphene/SiC compared to AlN grown directly on SiC (Figure 1). However, the success of this epitaxial growth is strongly dependent on the uniformity of a high-quality graphene monolayer on the SiC substrate.

Remote Epitaxy of GaAs and other III-V materials presents different challenges. While SiC has a well-developed graphitization process, high-quality graphene growth on GaAs remains elusive. In the literature, CVD growth of amorphous carbon has been explored as a 2D substitute for graphene. An equivalent fully MBE process has not yet been demonstrated and would enable in situ MBE Remote Epitaxy. We demonstrate epitaxy through amorphous carbon films; however, growth is dominated by pinholes due to film morphology (Figure 2).

To corroborate our experimental results, we employ DFT modeling to elucidate Remote Epitaxy in the context of island sliding energy barriers during the early stages of growth. Additionally, Kinetic Monte Carlo simulations are utilized to assess pinhole defects in 2D materials and evaluate relative contributions of lateral overgrowth versus Remote Epitaxy.

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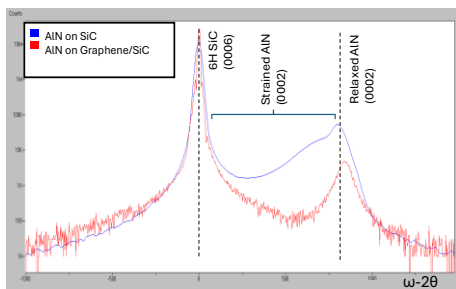


Figure 1. Reduced strain in Remote Epitaxial AlN on SiC

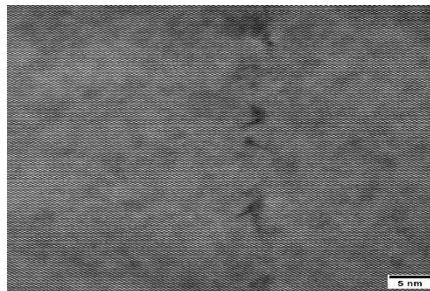
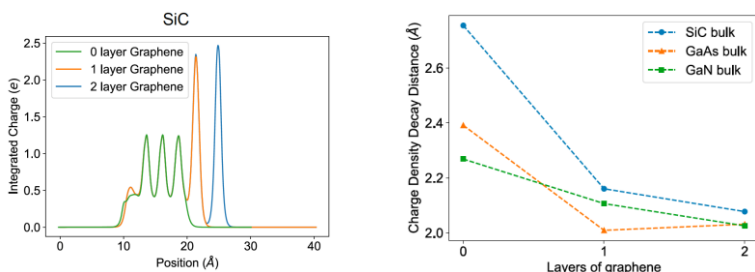


Figure 2. Epitaxial growth through perforated amorphous carbon MBE films

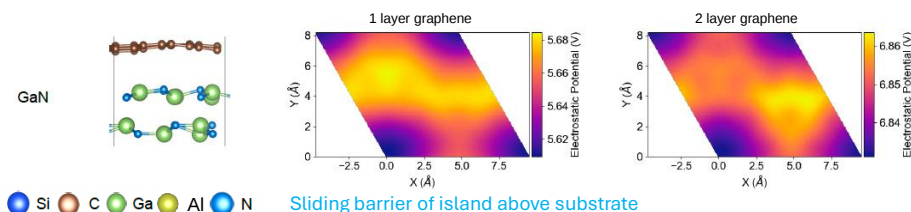
⁺ Authors for correspondence: swschmu@sandia.gov and jkoepke@sandia.gov

Supplementary Pages

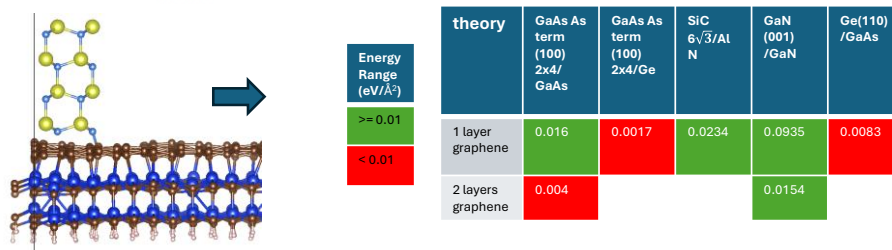
Charge Density Extension



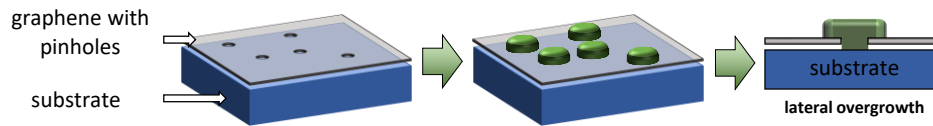
Electrostatic Potential 3 Å above substrate



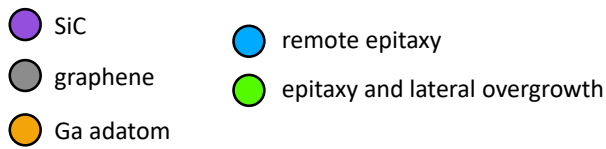
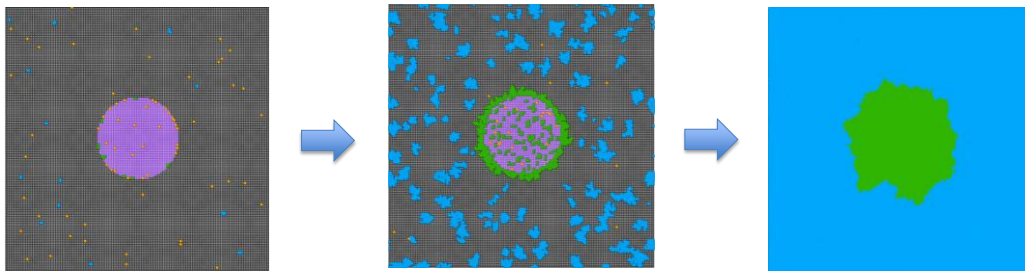
Sliding barrier of island above substrate



- **Problem:** Can we identify a metric using first principles calculations which lets us predict which substrate/film pairs would be successful for Remote Epitaxy?
- Previous explanations such as charge density extension and electrostatic potential above the substrate do not provide sufficient explanatory power
- The sliding Energy barrier of an island on the graphene surface appears to best predict epitaxy. Implies that kinetics of growth might be strong determinant of final success



- **Problem:** Real graphene and real substrates are never defect free. Consequently, any growth may be a combination of remote epitaxy and pinhole-mediated overgrowth
- A Kinetic Monte Carlo model employing energies from DFT calculations is used to predict the relative contribution of remote epitaxy and lateral overgrowth in Ga deposition on graphitized SiC substrates.



- Contributions from lateral overgrowth increase not only as a function of defect size, but also as a function of growth temperature.

