Atomic-Scale Mechanisms of III-V/Si Heteroepitaxy: From Nucleation to Defect Formation

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Abstract :

The monolithic integration of III-V semiconductors with group IV materials represents a transformative opportunity for integrated photonics, high-efficiency solar cells, and quantum devices. Since the pioneering work of H. Kroemer in the 1980s [1], fundamental challenges, such as lattice mismatch, dislocation nucleation, and thermal expansion disparities, have persisted as critical barriers to seamless III-V/Si heteroepitaxy. Despite decades of progress, these issues remain at the heart of contemporary efforts to achieve defect-free, co-integrated material systems.

Recent experimental findings, however, have challenged conventional interpretations of these growth mechanisms [2]. In this work, we integrate advanced epitaxial techniques, in situ microscopy, and Density Functional Theory (DFT) to investigate the role of surfaces and interfaces in governing Volmer-Weber growth of III-V monodomain islands on Si. Our combined theoretical and experimental approach enables us to predict and directly observe the equilibrium shapes of these islands in real time. Furthermore, we analyze their influence on antiphase boundary (APB) formation and propagation [2–8], providing new insights into defect mitigation strategies for next-generation heteroepitaxial systems. This research was supported by the French National Research NUAGES (Grant no. ANR-21-CE24-0006) and PIANIST projects (Grant no. ANR-21-CE09-0020). The work was granted access to the HPC resources of TGCC/CINES under the allocation A0120911434, A0140911434, A0160911434 and A0180911434 made by GENCI.

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