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Intitulé : Advanced DFT modeling of surfaces and interfaces for the monolithic integration of III-V semiconductors on Si

Directeur de Thèse : PEDESSEAU Laurent et CORNET Charles

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RESUME DE LA THESE

This thesis explores the atomic-scale epitaxial growth mechanisms of III-V semiconductors on Si(001) for applications in photonics and energy, using density functional theory (DFT). However, direct epitaxy remains challenging due to defects such as anti-phase boundaries and misfit dislocations. To address these challenges, this work develops a first-principles framework based on DFT to calculate absolute surface and interface energies in III-V/Si systems, enabling a quantitative evaluation of wetting behavior and interface thermodynamics. GaP/Si is studied as a model system to analyze the wetting behavior, revealing that an inevitable passivation on Si prior to epitaxy promotes 3D Volmer-Weber growth. A theoretical model for APB formation is then proposed, identifying these defects as metastable features formed as a consequence of island coalescence. Additionally, an ab initio Wulff-Kaischew construction is implemented to predict the equilibrium crystal shapes showing good agreement with *in situ* TEM observations of GaP/Si epitaxial growth. Notably, a novel fictitious charge passivation on surfaces scheme is introduced to accurately compute interface energies, effectively eliminating difficulties and errors from complex surface reconstructions. This method is applied first to biaxially strained, and next to 90° misfit dislocations of GaAs/Si systems, revealing energetically favorable dislocation core structures with charge compensation. Furthermore, preliminary calculations of the electronic band structure of this heterostructure structure reveal the presence of midbandgap states, which are associated with both dislocations and interfaces. Overall, this work advances the atomic-scale understanding and control of III-V/Si integration, offering new tools for optimizing next generation multifunctional devices, while also providing a new perspective on these heterostructures.