Croissance des composés III-N et de leurs alliages : developpement des outils numériques pour l'optimisation de leurs propriétés

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Abstract

The optical, electrical and thermal properties of group III-N semiconductors make them excellent materials for numerous electronic and optoelectronic applications. The thesis focuses on their growth by molecular dynamics (MD) simulations, as well as the development of numerical tools to analyze the results and characterize their thin-film properties. Thermal properties, such as the thermal expansion coefficient and the diffusion coefficient on the GaN surface were calculated using a Stillinger-Weber empirical potential. MD simulations were carried out for the growth of GaN on a GaN substrate, optimizing deposition conditions (temperature, deposition rate,..). The results show that crystallinity and morphology improve at high temperatures, low deposition rates, and relatively low N/Ga ratios. The growth of InN on GaN provides insights into the lattice mismatch problem between the GaN substrate and the deposited InN layer. The optimized growth conditions were then applied to the growth of GaN/InGaN/GaN quantum wells. Simulations reveal that high temperatures and thick layers promote indium segregation. Finally, the structural analysis of different chemical compositions of InGaN layers suggests that phase segregation of InN with GaN occurs due to strain relaxation, with indium-rich zones aligning along the growth direction [0001] in the form of columns. This work offers a numerical approach that provides insights into the growth and properties of III-N materials at the atomic scale.