

Interface characteristics in variant heteroepitaxial systems

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要旨

Various techniques associated with transmission electron microscopy have been applied to study the heterophase interface structure at an atomic scale. Interface structures have been classified into three types. (1) Formation of periodic mismatch dislocations, and formation of dimensionally uniform and nanoclusters. Such nanoclusters are quite similar to the quantum dots in conventional semiconductors as far as the dimensions, geometric shape and composition are concerned. (2) Thickness-dependent structural transformation. We clarified the nature of the thickness-dependent structural transformation in AlN film. The non-equilibrium cubic AlN, which normally exists under high pressures of more than 22.9 GPa, can be epitaxially stabilized in ambient atmosphere in the form of thin films grown on TiN substrate. A critical thickness, about 1.95 nm, at which the pseudomorphic growth cannot be preserved and after which the cubic phase transforms into its hexagonal counterpart, has been quantified. By means of the crystal-chemical atomic dynamics based on the first-principles calculations, we provide in-situ physical details in an atomic scale on the thickness-dependent structural transformation, which are hardly observed in experiments. (3) Formation of oriented domains in CMR films. Electron micro-diffractions and high-resolution imaging reveal that the La_{0.8}Sr_{0.2}MnO₃ thin film with thickness of 200 nm is epitaxially grown on the SrTiO₃ (001) substrate. The microstructures in the whole film are clarified in terms of the oriented micro-domains. Crystallographic relationships of these domains are discussed on the basis of an orthorhombic unit cell. Theoretical calculations based on a geometrical model that was recently proposed and applied to a number of epitaxial systems have been carried out to rationalize the present observations.