Ab initio and scanning tunneling microscopy study of indium-terminated GaAs(100) surface: An indium-induced surface reconstruction change in the c(8×2) structure

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Presentation 2 Abstract: Adding a small amount of indium (about 1 ML), which causes an In-stabilized c(8×2)-reconstructed (100) surface on the heteroepitaxial III-V growth front (e.g., InP/InGaAs and InAs/GaSb), has been found to improve the properties of these interfaces for electronics devices. In addition, it has been found that the In-stabilized c(8×2) surface can act as a potential starting substrate for producing insulator/III-V interfaces for future MIS transistors. In order to exploit the useful In-prelayers in the heteroepitaxial growth of III-V device materials, it is essential to understand the atomic structure of these In/III-V(100)c(8×2) surfaces.

We have studied the indium-terminated c(8×2)-reconstructed GaAs(100) substrate surface by the means of first-principles calculations and scanning tunneling microscopy (STM) measurements. Our total energy calculations demonstrate the stability of four different so-called ?a structures with In monomer rows and the In coverage between 0.5 and 2 monolayers (MLs) on the GaAs(100) substrate. Thus, we introduce III-V a surface system, which stabilizes the ?a reconstruction. The stability of the ?a reconstruction for any III-V semiconductor surface has not been confirmed theoretically before. Furthermore, we present an interesting trend. Atomic structure of the c(8×2) reconstruction depends on the surface layer cation and substrate volumes, which in principle allows to tune the surface structure by cation adsorption. This phenomenon is related to the unusual c(8×2) atomic surface structure, which shows mixed surface layer, including both anions and cations, and uncommon metallic type cations in the ?a structure, which do not show covalent bonds. Our results predict a structural transition from the ? structure to the ?a structure as the cation size is increased at 0 K. The found transition is probably related to the disordered surface structures (consisting of ? and ?a building blocks) found experimentally by x-ray diffraction at room temperature. Comparison of the STM images, calculated for various c(8×2) models, with the former and present measured STM images of In/GaAs(100)c(8×2) supports the presence of stable ?a reconstructions.