

Abstract

In the present work, the atomic surface structure of Si(100) and Ge(100) surfaces prepared in metalorganic chemical vapor phase deposition (MOCVD) ambient was studied with regard to subsequent heteroepitaxy of III-V semiconductors on group IV(100) substrates. At the crucial interface between the group-IV substrate and the III-V layer, single-layer steps on the substrate surface induce anti-phase disorder in the epitaxial film. In principle, double-layer stepped substrates can be employed to avoid anti-phase disorder. The MOCVD process gas environment strongly influences the domain and step formation of Si(100) and Ge(100) surfaces. To this end, in situ reflection anisotropy spectroscopy (RAS) and several other ultra-high vacuum-based (UHV) surface sensitive methods were applied to investigate the different surfaces dependent on the preparation. In situ RAS enabled identification of the surface structure and correlation of the crucial process steps, leading to complete control of surface preparation, in particular the domain formation of Si(100) and Ge(100) surfaces. Both the Si(100) and Ge(100) surface strongly interact with H₂ process gas which eventually leads to monohydride termination of the surfaces during preparation. Detailed analysis of Si(100) surfaces and the influence of the main process parameters indicated Si removal during processing in high H₂ pressure ambient. The generation of vacancies on the terraces induces a kinetically driven surface structure based on diffusion of vacancies and Si atoms leading to energetically unexpected step structures. Consequently, anomalous D_A-type double-layer steps, with dimers on the terraces oriented perpendicular to the step edges, are formed on vicinal Si(100) substrates according to in situ RAS and scanning tunneling microscopy (STM) measurements, whereas Si layer-by-layer removal occurs on large terraced substrates. However, processing in low H₂ pressure ambient leads to a step and domain structure which is energetically driven. In contrast to Si(100), H₂ annealed vicinal Ge(100) surfaces indicate no direct influence of the H₂ process gas ambient on the step structure. At the Ge(100) surface, group-V elements strongly influence step and domain formation as well as subsequent III-V nucleation. In this work, the exposure of vicinal Ge(100) substrates to As and P was studied. Detailed characterization of Ge(100):As surfaces showed the formation of single domain surfaces with different majority domain and significantly different step structures depending on temperature and As source, respectively. In contrast, exposure to P by annealing in tertiarybutylphosphine leads to a very disordered P-terminated vicinal Ge(100) surface according to low energy electron diffraction (LEED) measurements. In situ RAS measurements showed that the Ge(100):P surface is less stable compared to the Ge(100):As surfaces. The subsequent III-V heteroepitaxy strongly depends on the step and the domain structure of the group-IV(100) substrate. Here, RAS was established as a powerful in situ method to control all process steps of Si(100) and Ge(100) surface preparation in MOCVD ambient.