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Evan M. Anderson, Joanna M. Millunchick

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Interactions between Sb and As on InAs(001) surfaces

Evan M. Anderson and Joanna M. Millunchick

Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109-2136

Abstract

Interfacial broadening that occurs due to intermixing of Sb and As at the interfaces is a challenge for growing high quality mixed anion heterostructures. In this work, we examine the atomic scale interaction between As and Sb. Experimental observations show that the surface consists primarily of (4x3) and c(4x4) reconstructions as a function of As and Sb overpressure. Density functional theory calculations confirm the experimental phase diagram and show that many of the reconstructions contain both Sb dimers and sub-surface Sb. This indicates concurrent mechanisms for interfacial broadening: some Sb atoms are weakly bound in dimer sites and segregate during growth, while some Sb atoms are driven to infiltrate the crystal and intermix with As. The calculations also predict a stoichiometric Sb-terminated $\alpha 2(2 \times 4)$ to be stable, suggesting that abrupt III-As/III-Sb heterostructures could be obtained by growing on this surface. While not trivial to achieve, this surface can be experimentally obtained by depositing Sb directly on an In-terminated surface.

Keywords

A1. Surface Structure; A1. Phase Diagrams; A3. Molecular Beam Epitaxy; B1. Antimonides; B2. Semiconducting III-V Materials

I. Introduction

InAsSb and III-As/III-Sb compound semiconductor superlattices are materials of interest for mid wavelength and long wavelength infrared devices. However, high quality synthesis of these materials is complicated by the complex interaction between As and Sb. For instance, As is commonly observed to displace Sb at typical growth temperatures [1–7]. The opposite effect, Sb-for-As exchange, has also been reported under certain conditions in GaAsSb [5] and InAsSb [8]. Reports that Sb surface segregates in InAsSb are also common [9–12]. Indeed, this segregation has been thought to be the cause of the widely observed interfacial broadening in III-As/III-Sb heterostructures where Sb is unintentionally incorporated into the arsenide layers [4,9,11–16]. Interfacial abruptness can be improved by exposing the Sb-terminated layer to an As overpressure before growing the arsenide film, which is thought to displace excess Sb atoms [2]. However, prolonged As exposure has been shown to roughen the surface, since As is driven into the Sb-rich crystal [17]. Including atomic-scale details provides a more subtle understanding of this broadening; Sb displacement of As has been demonstrated to roughen the surface of InAs through a process driven by a surface

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