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The atomic surface structure of Bi-terminated GaAs(001) grown by Molecular Beam Epitaxy

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Abstract: Bi deposition onto GaAs surfaces changes the surface morphology, including smoothing the surface and anisotropic step growth. Bi also changes the surface reconstructions. Tiedje et al. (1) has observed that the GaAs(001) surface changes to a (1x3) reconstruction when Bi is deposited as a surfactant. Wixom et al. observed that Bi affects Ga adatom surface diffusion and incorporation at step edges (2). However, details of the (1x3) atomic structure and how it produces these effects have yet to be determined. Two series of GaAs samples were grown by molecular beam epitaxy for subsequent Bi deposition. Pure GaAs buffer layers were grown at a substrate temperature of 585C, after which the temperature was dropped to 415C for one series and 445C for the other. As overpressure was 5.5E-6 torr. The initial GaAs substrate exhibits a c(4x4) reconstruction according to reflective high energy electron diffraction (RHEED). The substrate was exposed to a Bi flux of ~1.5E-7 torr under no As overpressure as measured by a beam flux gauge and deposited in 1s increments, depositing 1-5s of Bi on a given sample. Upon exposure to Bi, the c(4x4) pattern evolved into a (2x3) followed by a (1x3) as Bi exposure time increased. Atomic Force micrographs of these surfaces show a marked decrease in the roughness with Bi layer thickness. Scanning tunneling microscopy images of the Bi-terminated GaAs surfaces show the atomic structure is a combination of several reconstructions reminiscent of the atomic surface structure of InGaAs alloys (3). Small regions of very regular 2(2x4) are clearly observed on the surface for both substrate temperatures. The presence of the (2x4) has been observed by Ahola-Tuomi et al. (4) and Laukkanen et al. (5) as a result of W-coil evaporation, however, in those instances the reconstruction was an 2(2x4) having one less group V dimer. The majority of the surface was covered in a less ordered reconstruction consisting of somewhat meandering rows running along the [1-10]. The spacing of these rows ranges in spacing between 0.99nm and 1.10nm, corresponding to an average spacing 2.6 time the bulk lattice spacing of GaAs along the <110>. Density Functional Theory (DFT) has also been applied in order to determine the structure of the reconstructions. In order to simulate the observed structure, (4x3) and ?(4x3) reconstructions, not typically observed for GaAs(001), were imposed and Bi systematically substituted for surface As atoms. Bi substitution on the 2(2x4) and 2(2x4) GaAs reconstructions was also pursued in order to compare the calculated surface energies.

References:

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