Isoelectronic doping atoms in III/V materials studied at the atomic scale by cross-sectional scanning tunneling microscopy

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To advance the semiconductor growth technology of novel highly mismatched III-V compounds, such as dilute nitrides, bismides and borides, atomic scale investigations of these materials are highly desired. Building on our experience with dilute nitrides [1,2,3,4] we focus in this presentation especially on a study of dilute bismides and borides. We will address several important issues in InP:Bi, GaAs:Bi, InAs:N and GaAs:B by cross-sectional scanning tunneling microscopy (X-STM). By combining high-resolution filled and empty state X-STM images with density functional theory (DFT) calculations, isoelectronic Bi_V and B_{III} atoms up to the several monolayers below the {110} III-V surfaces are uniquely identified and compared with results we obtained on isovalent N_V atoms in GaAs. We will present spectroscopic and voltage dependent topographic measurements of the Bi_V, B_{III} and N_V induced resonant state in the valence or conduction band and compare them with the atomic scale charge redistribution calculated within the Tight Binding (TBM) formalism and DFT. The results give a unique insight in the atomic properties of isovalent atoms in III-V materials.

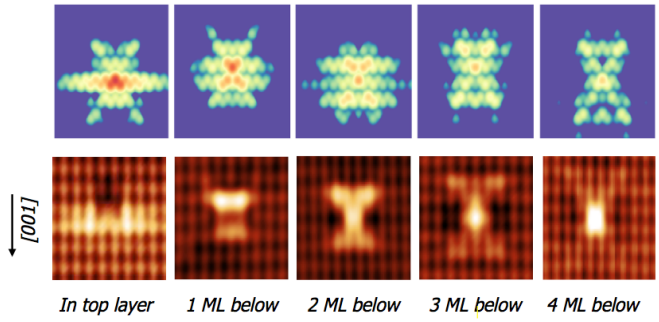

Fig. 1 Charge redistribution as measured around individual N_V-atoms in in GaAs at different depths below the cleaved surface (lower panels). Calculated charge redistribution (upper panels) for the experimental cases shown in the lower panels [2].

Based on the classification of these isovalent impurities, the structural properties of bulk doped layers and thin multilayer films are investigated. A clear trend for first neighbor pair formation is found for Bi in InP [5]. We observe that pairing for N and B in GaAs is less apparent. In areas with the highest Bi concentrations, we found that in addition to first neighbor Bi pair formation also Bi clustering occurs in InP.

Next to the expected lattice positions for B, N, and Bi we found additional defects such as cation vacancies and an additional class of atomic structures, which are tentatively identified as isoelectronic Bi_{In} anti-sites [5,6].

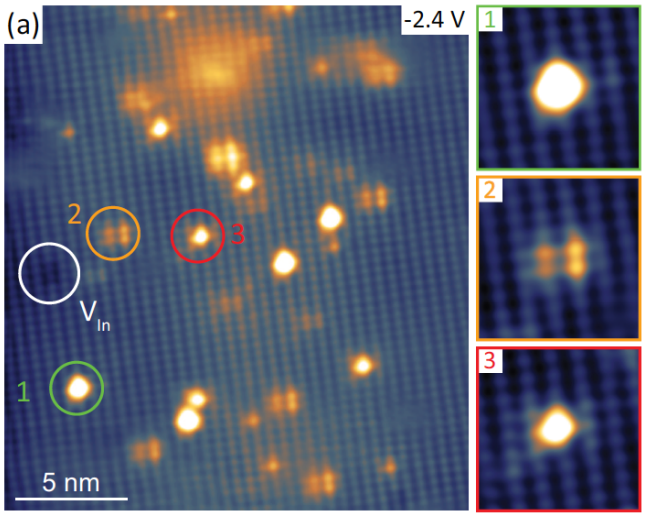

Fig. 2 Cross-sectional STM image of a cleaved Bi doped InP sample. We can directly observe the spatial distribution of Bi_V isovalent doping atoms up to 3 monolayers (panel 1,2,3) below the cleavage surface [5].

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