Cross-Sectional Scanning Tunneling Microscopy of Bi Atoms in InP

C. Krammel [1], K. Wang [2], Y. Gu [2], L. Y. Zhang [2], Y. Y. Li [2], Y. X. Song [2], Q. Gong [2], S. M. Wang [2,3] and P. M. Koenraad [1]

[1] *Department of Applied Physics, Eindhoven University of Technology, Eindhoven 5612 AZ, The Netherlands*
[2] *Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai 200050, China*
[3] *Department of Microtechnology and Nanoscience, Chalmers University of Technology, 41296 Goteborg, Sweden*

With the demand for low band gap materials (1 eV) for applications in high efficiency multijunction solar cells, isoelectronic co-doping with N and Bi in III-V compounds has recently attracted much attention [1]. Isovalent N doping provides a large band gap lowering [2] but suffers from low electron mobility [3]. A promising alternative is Bi doping, which does not affect the electron mobility whilst lowering the band gap effectively. Up to now few structural studies on Bi-doped III-V compounds have been performed [4].

We present a study on Bi-doped InP with cross-sectional scanning tunneling microscopy (X-STM), which, thanks to its unparalleled spacial resolution, is an ideal tool for such an investigation. The investigated sample was grown with molecular beam epitaxy and consists of a 420 nm thick (1.2 ± 0.2) % Bi-doped layer, which is separated from the Fe-doped InP substrate by an undoped InP layer of 70 nm. All X-STM measurements were performed on in situ cleaved (110) surfaces under UHV conditions ($p < 10^{-11}$ Torr) in an Omicron STM1 at room temperature.

In the atomically resolved filled state image (Fig. 1) can be four different types of Bi-related structures identified, which have not yet been observed or theoretically predicted. The bright features (A), which partially extended over their neighboring atoms, are associated with Bi_P substitutional impurities in the top layer. Similar features (B), with less contrast and an asymmetry with respect to their nearest neighbors along the [001] direction, are considered to originate from Bi atoms in the third layer below the cleaved surface. In contrast to these point-like structures (A) and (B) we also observed much weaker features that extend over two or more P sites. We classify these structures (C), which are oriented along the [1-10] direction, as belonging to a Bi atom in the second plane. Here, the large size difference between Bi and P atoms causes a significant outward relaxation of the two neighboring P atoms at the surface. Additionally, there are even weaker objects consisting of a square of four bright atoms (D), which are supposed to be from Bi atoms in the fourth layer. Significant hints for Bi clustering could not be observed. Current effort is undertaken to compare the Bi features with similar observations of individual N atoms in GaAs [5].

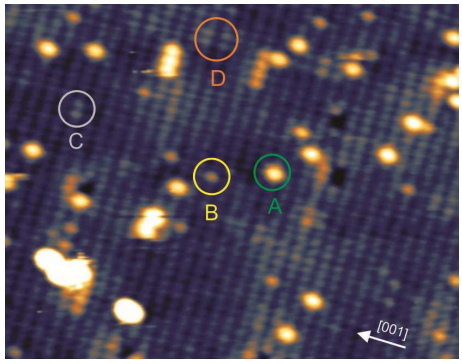

Fig. 1: Filled state X-STM image of Bi-related features A,B,C and D in InP taken at U= -2.7 V and I= 50 pA

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