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Quantitative STEM HAADF Analysis of Dilute Bi Containing GaAs

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Alloying conventional III/V semiconductors with elements with small or large covalent radius, like N or Bi, respectively, is important for several optoelectronic device concepts. While incorporating small amounts of N in III/V semiconductors leads to a reduction of the conduction band energetic position, the incorporation of Bi has a huge influence on the energetic position of the valence bands, mainly of the spin-orbit split-off band. However, the growth of such materials holds big challenges. To ensure a sufficent incorporation of Bi in GaAs, the growth temperature of metal organic vapour phase epitaxy (MOVPE)-grown samples has to be low. Because of such relatively low growth temperatures a good crystal structure is not necessarily guaranteed anymore.

We present the results of scanning transmission electron microscopy (STEM) high resolution high angle annular dark field (HAADF) measurements on MOVPE-grown Ga(AsBi)/GaAs quantum wells as well as on the quaternary material system Ga(NAsBi). We used a double C_S – corrected JEOL JEM 200 FS STEM with an annular dark field detector for the high resolution measurements as exemplarily depicted in figure 1(a). Modelling of scattered intensities is indispensible to quantitatively interpret such images. In this study, an absorptive potential approximation based simulation software (HREM [1]) was used for HAADF simulations. Especially for alloys containing atoms with highly different atomic parameters compared to those of Ga and As, like Bi, the simulation has to take realistic crystal models with static atomic displacements (SAD) into account. SADs were calculated using valence force field methods.

The evaluation of the HAADF measurements was performed with a Voronoi map based method by measuring the mean intensity of each atomic column. Thereto, the experimental image is divided in particular regions (for example Voronoi cells), where each cell contains one atomic column and a certain amount of pixels. One derives the mean intensity of each cell and hence of each atomic column by normalizing the cell intensity by the pixel number. It will be shown, that the construction of such a map allows to separate the group III and group V sublattices in the experimental and simulated HAADF images (figure 1(b)). Thus one can distinguish between atoms with nearly the same atomic number Z, such as Ga and As. Due to the sublattice separation it is also possible to determine the composition of each atom column, so that one can investigate the influence of Bi on the crystal structure by evaluation of the group V sublattice intensities only and in addition show the occurance of possible antisite defects.

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The present contribution will show how to gain information of crystal stochiometry and composition out of experimental as well as simulated HAADF images by constructing a mean intensity map. It will be shown that it is possible to describe the influence of local defects on an atomic scale quantitativley and give an outlook to the “new” material system Ga(NAsBi).

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[1] Ishizuka, K. (2002). A practical approach for STEM image simulation based on the FFT multislice method. *Ultramicroscopy*, *90*(2-3), 71-83

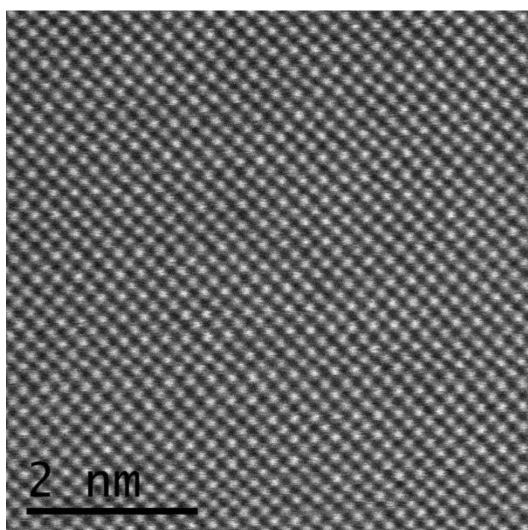

Figure 1(a): STEM HAADF image of a MOVPE grown Ga(AsBi) quantum well in [010] direction.

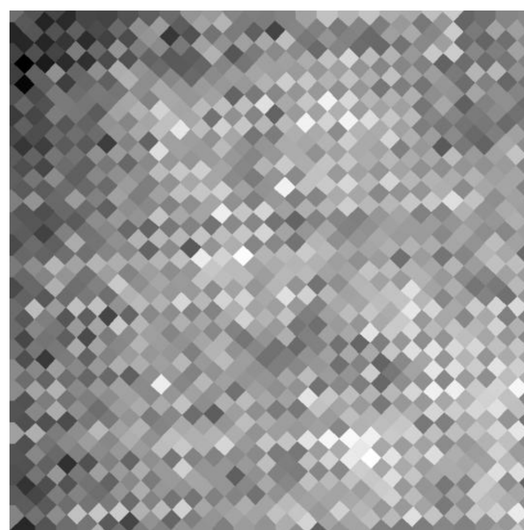

Figure 1(b): A mean intensity map (Voronoi map) of figure 1(a), which makes it possible to seperate the group III-from the group V-sublattice.

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