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*Determination of Bi positions in GaAs(1-x)Bi<sub>x</sub> heterostructures with atomic column resolution*

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**Abstract:** Aberration-corrected High Angle Annular Dark Field – Scanning Transmission Electron Microscopy (HAADF-STEM) provides Z-contrast (chemical sensitive) images with sub-angstrom resolution. Heavier atoms induce brighter contrast in the image, allowing the precise characterization of their position and distribution within a lighter matrix. Furthermore, with the help of image simulations, it is possible to quantitatively extract chemical information from III-V heterostructures[1] at atomic-column level.

The present work aims to study the distribution of Bi atoms in a GaAs(1-x)Bi<sub>x</sub>/GaAs heteroepitaxy from high resolution HAADF-STEM images. A sample grown by Molecular Beam Epitaxy (MBE) with a 2.65% Bi content[2] is studied in this work. Images were taken in a fifth-order spherical aberration corrected NION UltraSTEM electron microscope, working at 100 kV. In order to identify the best experimental conditions for a correct interpretation of the images, simulation is needed. From a simulated GaAs supercell with a thickness of 40nm, a number of As atoms at different <x,y,z> positions have been replaced by Bi atoms. Taking into account the potential electron channelling effect, Bi atoms were directly allocated to have 1, 2 or 3 atoms per column, depending on the Bi concentration considered. SICSTEM simulation software has been used in order to generate the resulting simulated images.

Simulation results show a direct relationship between intensity and Z in a certain range of values, being detectable the number of atoms in certain columns for a specific range of thicknesses. Bi atoms distribution is estimated from the analysis of experimental aberration-corrected STEM-HAADF images.

[1] S.I. Molina, D.L.Sales, P.L. Galindo, D. Fuster, Y. González, B. Alén, L. González, M. Varela, S.J. Pennycook, Ultramicroscopy 109, 172-176, (2009).

[2] M. Henini, J. Ibanez, M. Schmidbauer, M. Shafi, S. V. Novikov, L. Turyanska, S.I. Molina, D. L. Sales, M. F. Chisholm, J. Misiewicz, Appl. Phys. Lett 91, 251909, (2007).