Low and High resolution Parallel Software for HAADF-STEM Image Simulation

J. Pizarro[1], P.L. Galindo[1], M.P. Guerrero-Lebrero[1], A. Yañez[1], E. Guerrero[1], G. Scavello[1], F.J. Maestre-Deusto[1], D. Araujo[2], S.I. Molina[2]

[1]Dept. Lenguajes y Sist. Informáticos,
[2]Dept. Ciencia de los Materiales e I.M. y Q.I., Facultad de Ciencias
CASEM, Campus Río San Pedro, Universidad de Cádiz, Puerto Real-11510, Cádiz, Spain
joaquin.pizarro@uca.es

High Angle Annular Dark Field Scanning Transmission Electron Microscopy (HAADF-STEM), also known as Z-contrast is obtained by scanning an electron probe of atomic dimensions across the specimen and collecting electrons scattered to high angles. HAADF images are relatively immune to defocus and/or thickness effects contrary to an image obtained with a conventional transmission electron microscope (CTEM). They are also more sensitive to elements with large atomic numbers than those with small Z's providing chemical information at the nanoscale. A widely used methodology for precise atomic structural and composition analysis consists on comparing simulated images to experimental observations. This makes necessary the use of powerful image simulation tools for the research and study of nanostructures.

SICSTEM[1] is a parallel software code developed for running on the University of Cadiz Supercomputer (3.75 Tflops) that allows the simulation of high resolution images from large nanostructures containing more than one million atoms in reasonable time (from hours to a few days). The software has been designed to be able to generate not only one dimensional line scans or two dimensional images, but also to perform optical sectioning in the STEM simulation process. The input to SICSTEM software is a supercell described as a set of <x, y, z> coordinates for atom positioning, its composition, site occupancy, and Debye–Waller factor and the characteristics of the microscope: beam energy, third and fifth order objective aberrations, objective aperture, detector angles, etc. The image is simulated following a multislice[2,3] schema. We illustrate the results obtained by applying SICSTEM software to generate HAADF-STEM simulated image from an InAsP self-assembled nanowire. Specifically, an uncapped InAs quantum nanowire deposited by molecular beam epitaxy on an InP(001) substrate and periodically arranged along [110]. The z axis was defined as zone axis-crystal. The model was defined taking into account shape, compositions, boundary conditions and elastics parameters of the materials. The InP substrate was defined to be 8 nm high, the wetting layer 0.35 nm high and the wire was defined to be an isosceles triangle with two equal angles of 19,47º a side of 12 nm and 2.10 nm high. Model size was defined to be 18x15x10.45. Fig.1 shows the model and mesh used and the simulated image. The overall simulation process was 32 hours for a 575x982 pixels resolution image.

LowRes_SICSTEM is a low resolution HAADF-STEM software[4,5] based on the FFT multislice. For simulation purposes, the specimen is represented by a 3D arrangement of cubes where each cube is described by its chemical compositions, atomic density and atomic numbers. The probe, distributed in a Gaussian way, is set to an specified position (x,y,z) on top of specimen and illuminates the surface of several elementary volumes of the specimen which are inside the probe. The total intensity diffused at slice z is calculated as the weighted sum of all the n elementary cubes bombarded by electronic probe. This process is repeated slice by slice and the total intensity is computed by summing up contributions from all slices which determine the pixel intensity at each position in the image. The software has been implemented using the Jacket platform for CUDA programming[6]. CUDA is NVIDIA's parallel computing architecture and enables a significant increase in computing performance by exploiting the power of the GPU (graphics processing unit). For tomographic reconstruction purposes the software is able to generate 2D projections from the model at any desired angle. The results of applying this software to generate simulated images from 3D model of Cu and Ag precipitate on cubic geometry shape laying on a substrate of C is shown in figure 2.

References

[1] J. Pizarro, P.L. Galindo, E. Guerrero, A. Yañez, M.P. Guerrero, A. Rosenauer, D.L. Sales, S.I.Molina, Applied Physics Letter **93**, (2008) 153107
[2] K. Ishizuka, Microsc. Microanal. **10**, (2004) 34–40
[3] K. Ishizuka, Ultramicroscopy **90**, (2002) 71-83
[4] M. Shiojiri and H. Saijo, Journal of Microscopy, **223**, (2006), 172–178
[5] M. Shiojiri and T. Yamazaki, JEOL News, **38**, (2003) 54-59
[6] S. Ryoo, C. I. Rodrigues, S. S. Stone, J. A. Stratton, S. Ueng, S. Baghsorkhi, W. Hwu, J. Parallel Distrib. Comput. **68** (2008) 1389–1401

Figures

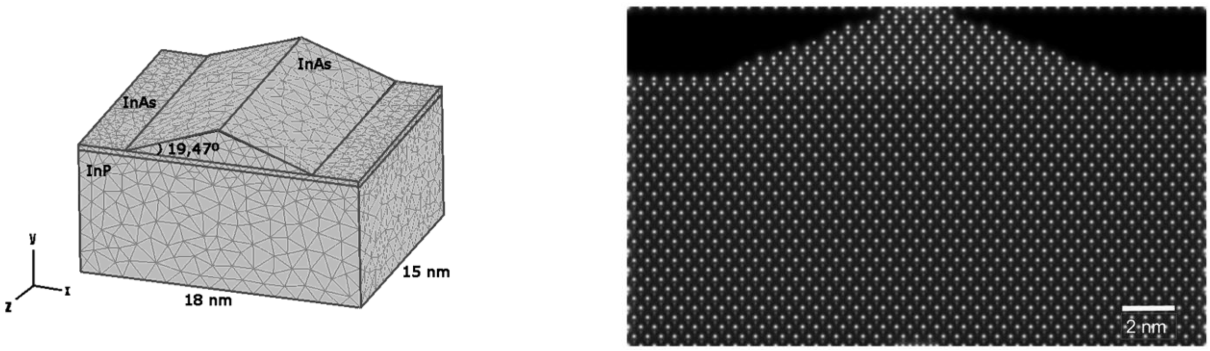

Figure 1: 3D InAs nanowire on InP sustrate model and simulated image.

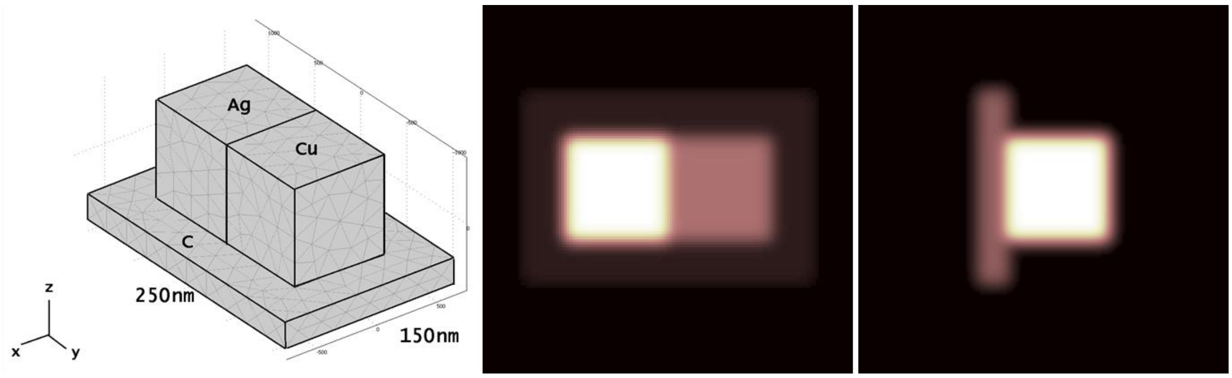

Figure 2: 3D model of Cu and Ag laying on a substrate of C and simulated images at two different projections (0 and 90 degrees around x-axis)