Parallel software for characterization of large nanostructures using HAADF-STEM

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Atomic resolution High-Angle Annular Dark-Field (HAADF) imaging in scanning transmission electron microscopy (STEM) is rapidly emerging as one of the most important techniques for the characterization of defects in materials. This technique is remarkably sensitive to the atomic number, being possible to generate images of small specimens at sub-Angstrom resolution in aberration-corrected microscopes. As it has been demonstrated recently [1], the measurement of spatial incoherence is important to detect interference effects of electron wave. The effect of spatial incoherence that occurs in electron microscopes produces a significantly lower contrast in experimental images [2]. This effect can be modeled by computer simulation using a convolution of the resulting image with a Gaussian envelope function, but a precise estimation of the incident electron wave is needed to interpret the final Z-contrast images. To maximize simulation precision, an approach to obtain the optimal width of the Gaussian function is presented in this work.

SICSTEM [3] is a parallel simulation software for the simulation of HAADF-STEM images of large nanostructures developed in our research group at the University of Cadiz. SICSTEM runs on a the CAI cluster composed of 80 nodes, each consisting of two Intel Dual Core Xeon 5160 and 8 MB of random access memory, being the overall number of cores equal to 80 x 2 x 2 = 320 and achieving a peak performance of 3.75 TFLOPS (1 TFLOP10^{12} floating point operations per second). It allows the image simulation of large supercells (thousand atoms) within a reasonable time (hours or a few days). SICSTEM takes into account thermal diffuse scattering (TDS) in the calculation of the intensity in the object exit plane by the multislice method using a local TDS absorptive potential approach and its accuracy has been successfully compared to Ishizuka's FFT multislice approach using the WinHREM™ software.

In this work, a new functionality to take into account the effect of spatial incoherence, to reduce the differences in contrast between experimental and simulated images (usually called Stobbs factor) [4] has been included in SICSTEM software. This correction consists on selecting a set of corrected simulated images with different standard deviations and compare them with experimental images using as figure of merit an expression based on the difference in contrast in Fourier space. The proposed functionality aims to be fixed for a given microscope (in the same conditions) and independent of the sample.

In order to show the feasibility of the method and validate its performance, a collection of experimental and simulation images have been used to calculate the effect of spatial incoherence. Experimental images were obtained using a 100kV dedicated VG Microscope HB501Ux STEM equipped with a Nion aberration corrector, Cs = - 50µm, C5 = 63mm, inner detector angle = 70mrad, outer detector angle =

200mrad and objective aperture = 27mrad. In this work, three compositions of InxAs1-xP (27%As, 59%As and 87%As) on a InP substrate and oriented along [110] have been analyzed [5]. For each composition, three different thicknesses have been studied, obtaining a total of nine images. Figure 1 shows error function to determinate the Gaussian function that simulates the effect of spatial incoherence for three As compositions. Figure 2 shows this error function for different thicknesses of InP. From these figures, we might conclude that the proposed method is independent of the composition and thickness of material. Experimental results after the correction have also shown an excellent agreement between simulated and experimental images.

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Figures

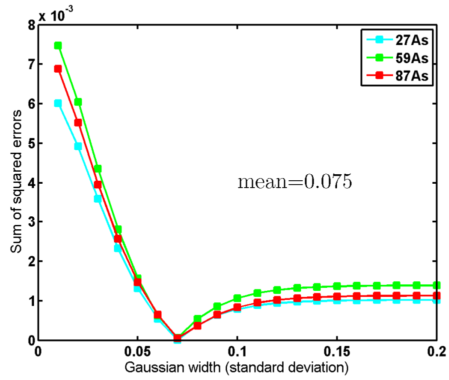

Figure 1.Error function to determine the Gaussian function that simulates the effect of spatial incoherence for three As compositions.

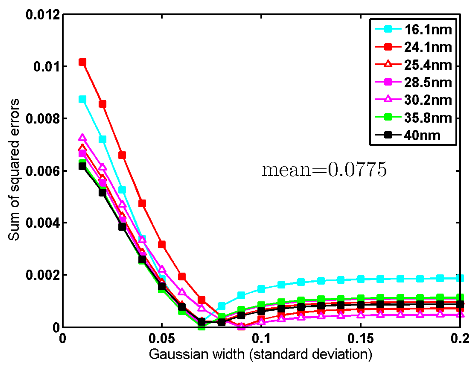

Figure 2.Error function for different thicknesses of InP. It is possible to conclude that the proposed technique is independent of material thickness.