Parallel software for the simulation of high angle annular dark field images at low magnifications

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This work presents a novel parallel low resolution High Angle Annular Dark Field Scanning Transmission Electron Microscopy (HAADF-STEM) software based on the multislice algorithm[1][2]. HAADF-STEM images, also known as Z-contrast, are obtained by scanning an electron probe of atomic dimensions across the specimen and collecting electrons scattered at high angles.

In the low resolution simulation approach[3] the specimen is represented by an arrangement of 3D cubes, where each cube is composed of some atoms and described by a set of parameters, such as its chemical composition, atomic density and atomic number.

The probe is set to an specified position (x,y,z) and illuminates the surface of the specimen.

The whole process consists on a sequence of transmission-propagation of the wavefunction across all the slices. The 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.

This simulation process has a high computational cost and therefore its use is limited to computer centers with large supercomputing systems. However, with the advent of GPUs, some tasks may be implemented in parallel and run in usual PCs. In this paper, we have analyzed three parallel alternatives to the usual sequential programming implementation.

For the first approach, all calculations are splitted into different threads and each one is run in a different core of the CPU. The second option is to call high-level programming specialized functions for GPUs. For the last approach, we do not divide the problem in blocks, but we make use of the philosophy of massive parallel processing present in the GPUs architecture.

To test the algorithm, we calculated the computational time of simulating several images at different resolutions of bulk boron-doped carbon (Figures 1 and 2). We can observe in figure 3 that the computation time is reduced exponentially using the GPU, and specially using the CUDA approach toolkit making possible the simulation of an image in a reasonable time in a personal computer without great economic effort.

Acknowledgments

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References

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[2] Ishizuka K. Ultramicroscopy 90 (2002) 71

[3] J. Pizarro et Al., Appl. Phys. Lett. 93 (2008) 153107

Figures

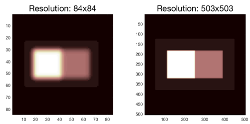

Figure 1: Bulk boron-doped carbon low resolution HAADF simulated electron microscopy images with a resolution of 84x84 pixels and 503x503 pixels

Figure 2: Simulation of a low resolution (100px) image projections from different angles (0°, 45° and 90°)

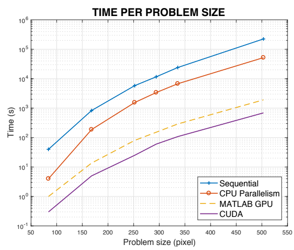

Figure 3: Time in seconds for each image resolution on an Intel Xeon CPU E5-2620 v2 with 12 cores and a NVidia Tesla K20c