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Recent Advances of the Open Source MULTEM Program to Provide Accurate and Fast Electron Microscopy Simulations

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Nowadays, modern transmission electron microscopy (TEM) is capable of reaching sub-Angstrom resolution in both TEM and scanning TEM (STEM) mode [1,2]. Furthermore, the microscope becomes less restricting and the quality of the experimental images is mainly set by the unavoidable presence of electron counting noise. However, due to the quantum mechanical nature of the electron-specimen interaction, images are no longer related to the specimen structure in a simple manner and therefore all experimental work needs to be complemented by numerical simulations.

The most practical method for TEM image simulations is the multislice method, which is known to be an accurate numerical procedure for solving the quantum mechanical electron-specimen interaction. In the multislice formulation, the specimen potential is divided into many slices perpendicular to the electron beam. Each slice is chosen thin enough to be considered as a weak phase object, modifying only the phase of the incident wave. The potential between two consecutive slices is considered to be zero and the propagation of the electron wave between the slices is approximated by the Fresnel propagator. The electron wave at any depth in the crystal can be calculated by using this process.

It is known that in order to match TEM experiments with simulations, inelastic scattering cannot be neglected and it has to be included in the simulations. Electron-phonon scattering is often incorporated by using the frozen phonon model [3]. The basic idea of this model is to perform repeated multislice simulations for different atomic coordinate configurations. Each configuration needs to be taken as the outcome of realistic phonon calculations or by using the Einstein model in which the atoms vibrate independently. The final image or diffraction pattern is the intensity averaged over the different configurations. The electronic excitations are usually included by using the density matrix approach under the assumption that a single inelastic event takes place on a single atom at a given depth [4].

The MULTEM program was developed with the purpose of performing accurate and fast multislice simulations for all different TEM experiments including high resolution TEM, electron diffraction (ED), precession ED, hollow cone imaging, convergent beam electron diffraction (CBED), convergent beam electron imaging, STEM, imaging STEM, energy filter transmission electron microscopy and STEM energy loss spectroscopy. MULTEM includes the phase object approximation (POA) and weak POA which provides qualitative description of the electron specimen interaction as well as the main atomic electron scattering parameterizations. In order to perform accurate simulations, we include the frozen phonon approach for the electron-phonon interaction, the density matrix approach for electronic excitations, correct inclusion of the spatial and temporal incoherences for plane wave and convergent beam illumination. To be able to perform fast simulations, MULTEM is optimized for computer cluster and GPUs which speed up the calculations between 2-3 orders of magnitude as compared with a desktop multicore computer [5].

In order to keep in touch with the latest instrumental development in the microscopy field where two-dimensional diffraction patterns are recorded for each scan position, also called 4D-STEM, we introduce

the multiprobe CBED calculations in which in one multislice run we can obtain several CBED patterns. This development allows one to speed up 4D-STEM simulations by a factor proportional to the number of beams as shown in Fig. 1.

Figure 2 shows an example of a frozen atom image calculation using an annular dark field aperture of an isolated heme-binding protein (HbpS) complex which contains 7976 atoms. In these simulations, plane-wave illumination is assumed with the following electron microscope settings: acceleration voltage (300 keV), spherical aberration (0.04 mm), defocus spread (32 Å), beam divergence angle (0.2 mrad), defocus (109 Å) and annular aperture (g_{min} = 0.5 $Å^{-1}$, g_{max} = 2.0 $Å^{-1}$). A numerical real space grid of 8192x8192 pixels has been used. The frozen atom simulation is performed by using the Einstein model with 200 configurations, slice thickness of 1Å and the three-dimensional rms displacements of all the atoms are set to 0.15Å. For the HRTEM simulation, the spatial and temporal incoherences are included by applying the partially coherent microscope transfer function to each exit wave of the frozen atom.

In this work, we have shown that accurate, fast and realistic simulations can be performed in a reasonable amount of time with the open source program MULTEM even for large structures [6].

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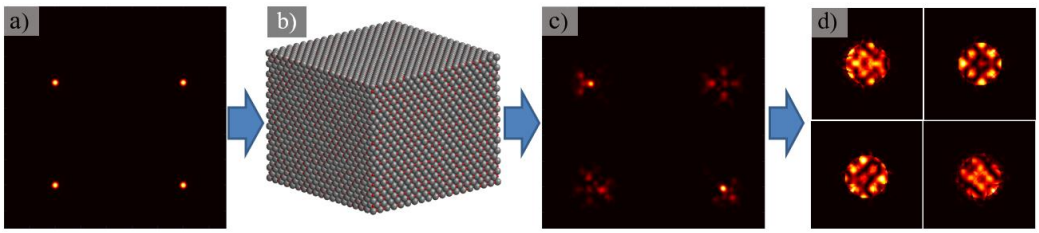

Figure 1. Schematic representation of the multiprobe CBED calculations. a) Incident multiprobe, b) specimen, c) wave function in real space and d) CBED patterns after applying a mask function.

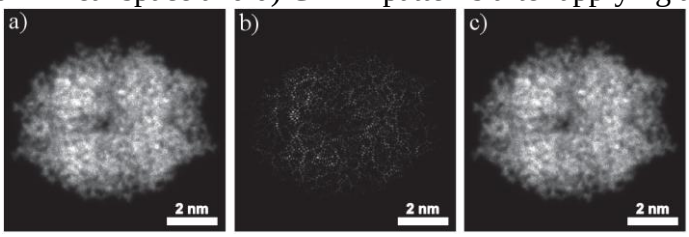

Figure 2. Frozen atom image calculation of a complex HbpS. a) Total intensity, b) coherent intensity (elastic) contribution and c) incoherent intensity (inelastic) contribution.

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