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Compressed STEM Simulations

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Over recent years it has been shown that high resolution scanning transmission electron microscopy (STEM) images can be acquired by directly subsampling the probe locations [1-2] and inpainting the missing information, so could similar methods be applied to STEM simulation? A common approach to STEM simulation is the multislice method [3,4], where the 3-dimensional atomic potential of a sample is approximated as a series of 2-dimensional slices. MULTEM [5] is one example of STEM simulation software which can accurately provide representation of electron transmission in a STEM [6] using this multislice method. To account for thermal diffuse scattering, the frozen phonon model [7] is used, which takes a snapshot of the sample at some given time where the atom locations are slightly displaced from their equilibrium position depending on the Debye-Waller factor [7] of the atom (figure 1(c)). Each snapshot of atom positions is known as a frozen phonon configuration (FPC) and the more configurations considered, generally the more accurate the simulation [5,7]. However, this method is computationally expensive and therefore requires either a high-end machine, and/or a long time to compute [8] to make sure the simulations have converged to best match the experiment. This approach also runs into severe limitations when the comparison experimental image quality is poor [9]. This means that if a material, interface, or defect is susceptible to electron beam damage, it is hard to develop precise simulations of these structures.

Our method to spatially compress a simulation is to first divide the output region into a set of discrete patches (figure 1(a)). Any desired sampling pattern can be generated by the user and then there is a function to call each required patch to be simulated. These patches are then substituted back into their respective position in the output region. This then provides a spatially sub-sampled simulation. Given that the dominant scattering process in HAADF STEM is incoherent, the maximum scattering angle can be limited to the outer diameter of the HAADF detector (figure 1(b)), hence fewer reciprocal space vectors are required for the output image. It is also possible to reduce the number of FPCs given that the increase in accuracy diminishes beyond some critical value. This critical value depends on the thickness of the sample, its vertical periodicity, and whether it contains any exotic properties such as grain boundaries or defects. The spatially subsampled simulations are reconstructed through an inpainting algorithm. Our inpainting algorithm consists of two key parts- a (blind) dictionary learning algorithm, followed by a sparse coding algorithm. The image recovery problem is turned into a Bayesian dictionary learning problem based on the Beta Process Factor Analysis (BPFA) developed in [10].

The results (figure 2(a)) show that it is possible to achieve over 90% structural similarity (SSIM) [11] with 3% spatial sampling, 5 FPCs, and a maximum reciprocal space vector of 5.12 $Å^{-1}$. In this presentation, the development towards real-time simulations will be discussed, which is the first step in the rapid interpretation, classification, and analysis of images and potentially the future development of artificial intelligent STEM [12].

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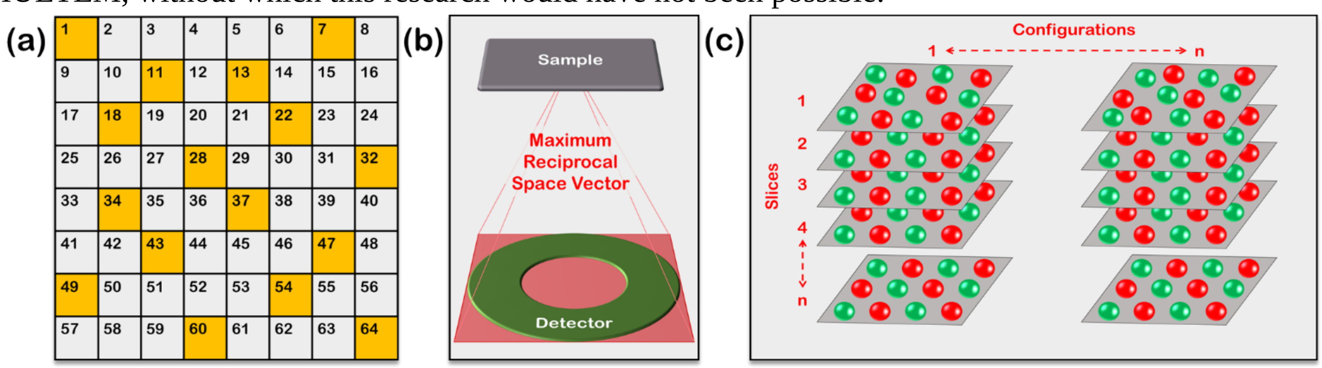

Figure 1. The three methods of simulation compression. (a) The simulation output space is divided into N patches of size [m x m] pixels. Each patch is indexed 1 to N (in this case N = 64) and the patches highlighted are called to be simulated, in this case a random 25% sampling mask. (b) The simulation space in red is limited to the outer diameter of the detector (green) and corresponds to the maximum reciprocal space vector used in the simulation. (c) A diagram showing the frozen phonon model approximation.

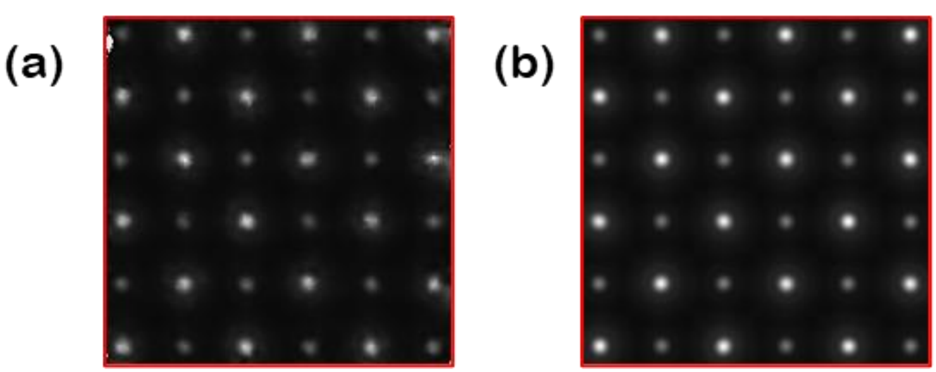

Figure 2. (a) Reconstruction of a compressed simulation of bulk SrTiO3 with 3% spatial sampling ratio. It has an SSIM of 92.6% and PSNR of 26.7 dB with respect to (b) the fully sampled simulation.

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