Incorporating Prior Knowledge for Atomic Resolution Tomography

K.J. Batenburg,* J.R. Jinschek,** H.A. Calderon,*** and C. Kisielowski****

* Leiden University, Mathematical Institute, P.O. Box 9512, 2300 RA, Leiden, The Netherlands and Centrum voor Wiskunde en Informatica, P.O. Box 94079, 1090 GB, Amsterdam, The Netherlands.
** Virginia Tech, Materials Science and Engineering, 309 Holden Hall (0237), Blacksburg, VA 24061, U.S.A.
*** ESFM-IPN, Dept. de Ciencia de Materiales, Mexico D.F., Mexico.
**** National Center for Electron Microscopy (NCEM), LBNL, Berkeley, CA 94720, U.S.A.

Over the past few years, electron tomography has become a valuable tool in materials science to investigate the three-dimensional structure of nanomaterials [1]. At present, the spatial resolution of electron tomography reaches towards 1 nm^3 [1,2]. A large number of images (>100) are required to compute accurate reconstructions.

Recently, we proposed a novel approach towards atomic resolution tomography, which makes use of zone axis images, obtained by TEM or STEM. The approach utilizes the fact that atoms are discrete and occur in columns in a nanocrystal. It has been demonstrated experimentally that if the sample is very thin (smaller than the first extinction oscillation), it is possible to count the number of atoms in each projected column [5]. If sufficient count data are available from several zone axis projections, then it is possible to reconstruct the 3D positions of the atoms of a nanocrystal using discrete tomography.

The two basic assumptions of this model - atoms are discrete and occur in columns - restrict the possible solutions that the reconstruction algorithm needs to consider. Therefore, far fewer projections are required compared to "conventional" electron tomography. In [5] it is shown that for a small test structure, consisting of 309 atoms, only six projections are sufficient to compute a perfect reconstruction, even in the presence of noise, i.e., atom count errors.

Once the atom count data have been collected, computing the actual reconstruction is not a straightforward procedure. The reconstruction problem is NP-hard, which in practice means that the computing time required to find a reconstruction may be exponential in the number of atoms. Another challenge for the reconstruction algorithm is non-uniqueness of the solution: there may be several atom configurations leading to the same measured projections [6].
Our algorithm [3], already utilized in [4, 5], is very general and does not utilize available prior knowledge of physical properties of the sample. To increase the probability of finding the correct atom configuration corresponding with the sample, we propose to use additional prior knowledge in the reconstruction step. However, it is also important to still allow for possible atom configurations that are very unlikely and occur rarely. A good method to model prior knowledge is to use a statistical model. Thereby, no hard constraints on the occurring atom configurations are imposed. Gibbs distributions are well suited for this task, as they can be defined locally [7,8]. Certain local atom configurations in a crystal that are physically impossible or highly unlikely are assigned very low probabilities. On the other hand, the configuration that corresponds to the regular crystal grid is assigned a high probability (see Fig. 1). The reconstruction algorithm will now search for a reconstruction that corresponds well with the measured projection data and is most likely according

to the Gibbs distribution. Note that this reconstruction may still contain rarely occurring local atom configurations, as the probability model does not impose any hard restrictions.
We will present several kinds of local prior knowledge that can be incorporated in the reconstruction algorithm, along with a scientific justification for the assumptions that are made. Gibbs priors are commonly used in image processing and several algorithms are available for computing the corresponding reconstruction. Experimental results, obtained with and without using prior knowledge, will be compared.

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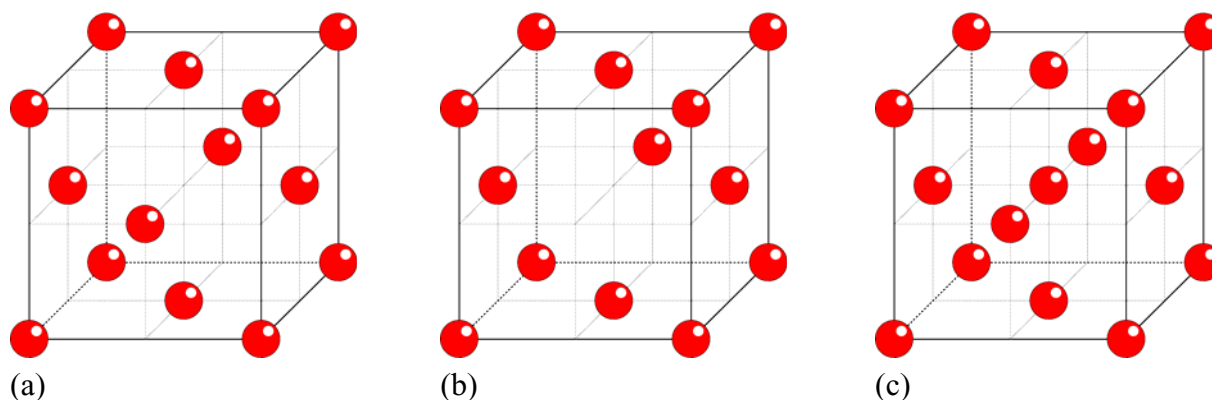(a)   (b)   (c)

Fig. 1. Three local atom configurations in a face-centered cubic (fcc) crystal lattice. Configuration (a) corresponds with the perfect crystal and is assigned a high probability in the statistical model. Configuration (b) represents a vacancy (center of the front face), which occurs far less frequently than configuration (a). Configuration (c) includes an atom in an interstitial position (center), which is highly unlikely if the crystal consists of only one type of atoms.