STRUCTURAL FINGERPRINTING IN THE TRANSMISSION ELECTRON MICROSCOPE

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Two novel strategies for the structurally identification of nanocrystals in a Transmission Electron Microscope (TEM) are described [1]. Either a single High-Resolution Transmission Electron Microscopy (HRTEM) image [2] or a single Precession Electron Diffractogram (PED) [3] can be employed. The structural identification information is in both cases collected on an individual nanocrystal. Automation of the method may lead to statistically significant results on a set of nanocrystals. The structural information that can be extracted from a HRTEM image of an approximately 5 to 10 nm thick nanocrystal is the projected reciprocal lattice geometry, the plane symmetry group, and a few structure factor amplitudes and phases. While the structure factor amplitudes suffer from dynamical diffraction effects and are in addition modified by the (not precisely known) contrast transfer function of the objective lens, the structure factor phases are remarkably stable against dynamical diffraction effects and slight crystal misorientations.
Except for the structure factor phases, the same kind of structural information can be extracted from a PED, but the information that can be used for structural fingerprinting is in this case not limited to the directly interpretable resolution of the TEM. As precession electron diffraction avoids crystal orientations that result in the simultaneous excitation of more than one strong diffracted beam (as much as this is possible), quasi-kinematic reflection intensities are obtained for nanocrystals with thicknesses up to approximately 50 nm. Simultaneously present reflections in high order Laue zones and systematic absences in both the higher and the zero order Laue zones allow frequently for an unambiguous determination of the space group [4]. (Comparing kinematical electron diffraction simulations with experimental PEDs allows, therefore, for structure verifications. While those higher indexed reflections that are not also higher orders of strong reflections can frequently be treated as kinematic, modest primary extinction of low indexed reflections can be corrected for following Blackman's seminal paper [5].)
Searching for structural information that is extracted from HRTEM images or PEDs in comprehensive databases and matching it with high figures of merit to that of candidate structures will allow for highly discriminatory identifications of nanocrystals, even without additional chemical information as obtainable in analytical TEMs.

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[5] M. Blackman, *Proc. Royal Society (London)* A **173** (1939) 68-82