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HRTEM contrast of nanoparticles embedded in a metallic matrix

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Melting, crystallization and e.g. mechanical properties of small particles are in focus of current research due to size effects. However, nanoparticles embedded in a matrix may show additional contributions to their properties caused by the character of the interfaces. In the present study, the contrast in high-resolution transmission electron microscopy (HRTEM) arising from metallic nanoparticles embedded in a metallic matrix are studied. It is the aim of the present work to explain moiré effects observed in experiments by image simulations using a multislice algorithm and a simple atomistic model.

Samples for the experimental observation of embedded nanoparticles were made using the melt-spinning technique. Aluminium bands with embedded indium nanoparticles were ion-milled using a Gatan PIPS with acceleration voltages between 3.5 and 1 kV. HRTEM images were made using an aberration-corrected Titan 80-300.

For the image simulations atom positions of a freestanding nanoparticle with a flat Al-matrix above were generated using the Mathematica™ software platform. An example of a generated ensemble of atomic coordinates is shown in Figure 1. For simplicity, the crystallographic orientation was always [100] parallel to the incident electron beam. The thickness of the matrix as well as the size of the nanoparticles were systematically varied. HRTEM images of the as-generated structures were simulated using the multislice algorithm by Kirkland [1]. To fit experimental conditions, the partial coherence of the propagating electron wave was included. Therefore, the acceleration voltage was set to 300 kV, with 1 mrad spread in illumination and a slightly negative Cs-value (thermal vibrations were not taken into account). Results of the simulation are shown in Figure 2. A matrix thickness of 1, 10 and 20 unit cells is simulated in (a), (b) and (c), respectively. A matrix of 10 unit cells with a larger spherical nanoparticle is shown in (d). The propagation of the electron wave through the matrix and the nanoparticle leads to a moiré pattern. The moiré intensity variation consequently leads to local regions where the lattice information of the matrix is dominant, and local regions were the lattice plane spacing of the nanoparticle can be seen almost entirely. At a similar thickness of the matrix and the particle this local contrast variation gets strong, leading to situations where parts of the nanoparticle apparently disappear (cf. arrow in Figure 2 (c)). For a larger particle the moiré pattern stays fairly homogenous across the particle, whereas the interface becomes artificially rough. Measured atomic distances show strong variations with the moiré pattern, making it difficult to obtain real atomic positions.

An experimental HRTEM image of an In nanoparticle in an Al-matrix is shown in Figure 3. The power spectrum is shown as an inset, where many moiré spots are visible. The moiré pattern in this HRTEM image is fairly uniform across the faceted particle, however, small variations of the orientation of the moiré fringes can be observed. Moreover, two missing wedges can be observed on two opposite sites of the particle. Intensity modulations due to the moiré effect possibly exterminate a weak contrast arising by atoms at corners of the nanoparticle.

As a conclusion it should be pointed out, that the spacing of the moiré pattern can be used to determine the difference of the involved lattice planes with a high accuracy, however, measurements of absolute atomic positions are not possible and even atoms and atomic columns can become "invisible" at local regions of the moiré pattern. Moreover, apparent interface roughening can occur by moiré effects. Therefore, image simulation is inevitable to interpret atomic positions at interfaces, in particular when a nanoparticle is embedded and not of constant thickness.

1. Kirkland, E. J. "Advanced Computing in Electron Microscopy" Springer (2010).

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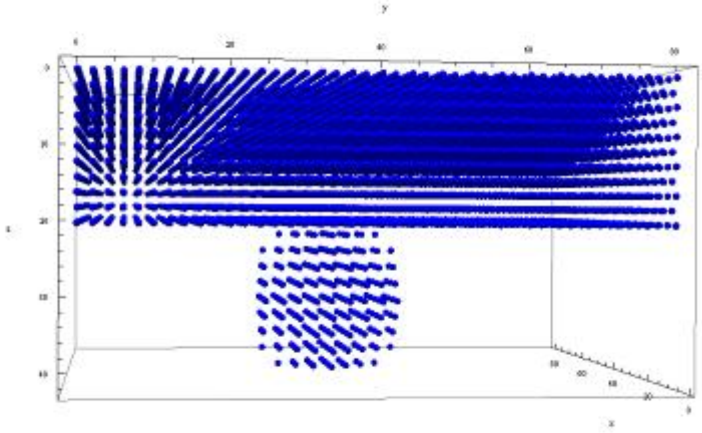

Figure 1. Simulation box of a matrix structure (on top) and an underlying nanoparticle (bottom). For the multislice simulation including partial coherence the size of the matrix as well as the size of the particle were varied. The nanoparticle is slightly facetted.

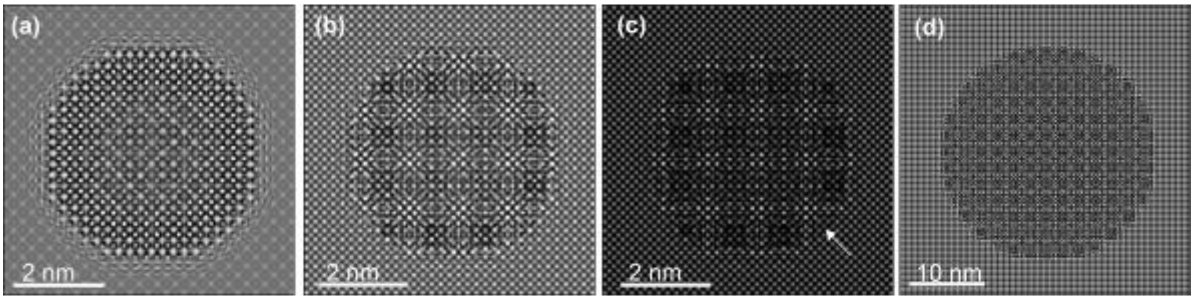

Figure 2. Multislice simulated HRTEM images of a nanoparticle and an Al-matrix. The thickness of the matrix was varied: 1 unit cell in (a), 10 unit cells in (b), and 20 unit cells in (c). The arising moiré pattern overlays the contrast of the atom columns. At a similar thickness of the matrix and the particle the local contrast of the nanoparticle gets weak, as marked by the arrow in (c). For a larger particle the moiré pattern stays fairly homogenous across the particle, whereas the interface becomes artificially rough.

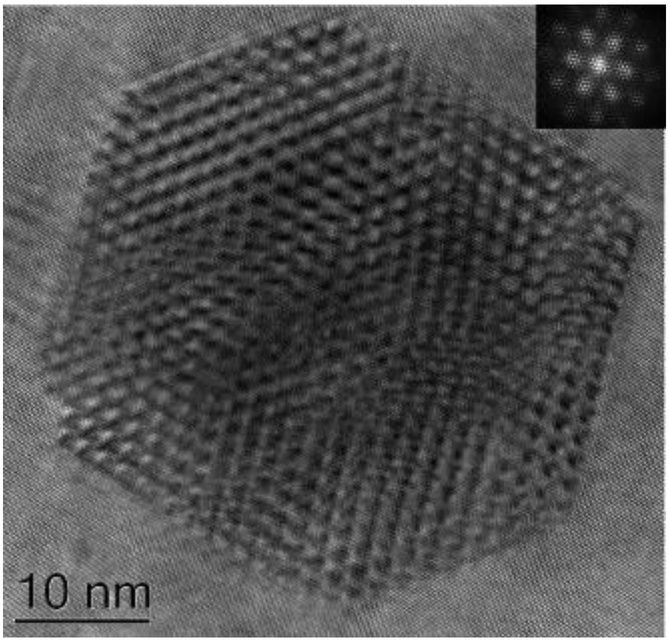

Figure 3. Experimental HRTEM image of an In nanoparticle in an Al-matrix, the insert shows the power spectrum. The moiré pattern is fairly uniform across the faceted particle. Two missing wedges can be observed on opposite sites of the particle. However, intensity modulations due to the moiré effect possibly exterminate a weaker contrast of atoms/atomic columns at corners of the nanoparticle.