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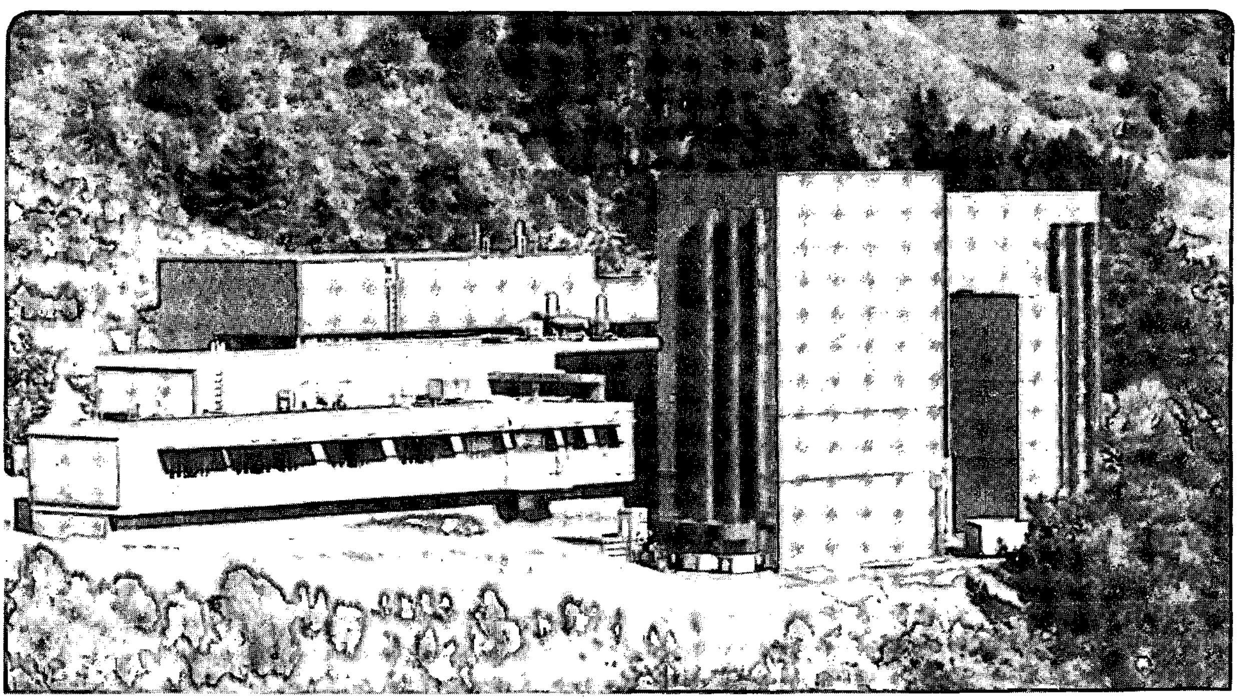

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THE EFFECT OF CRYSTAL TILT ON HIGH RESOLUTION MICROGRAPHS OF SMALL METAL PARTICLES

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INTRODUCTION

The structure of small (≈1.5-5.0 nm) metal particles has been studied extensively by high resolution transmission electron microscopy (HRTEM) [1,2,3 and refs. therein]. When imaging particles of this size it is not possible to use the tilting techniques (selected area diffraction) usually employed by the high resolution microscopist. This means that the microscopist often has to totally rely on the appearance of the image when deciding in which direction the particle is viewed. This work points out some of the problems of intuitive determination of the viewing direction.

METHODS

Image simulations of tilted metal particles has previously been performed [2,4] but most of them has so far been focussed on low index directions. The scope of this investigation is to do a comprehensive simulation study of the appearance of a tilted metal particle. As model particle a perfect five-shell (561 atoms) palladium cubeoctahedron (fig. 1) was chosen. The particle was placed free (no support) in a super cell (6*6 nm) and the simulations were performed with the NCEMSS package [5] using 256*256 sampling points. The microscope parameters used were those of a JEM-4000EX and the simulations were all calculated for a defocus of -50 nm (≈1.2 Scherzers). The tilting scheme is shown in fig. 3 where the position of the cubeoctahedron with respect to the coordination system used is given. The rotation axis, R, is defined by the angle ω and the amount of rotation is given by the angle α.

RESULTS

A map of tilted particles have been simulated with ω ranging from 0 to 90 degrees in steps of 10 degrees and α ranging from 0 to 45 degrees in steps of 5 degrees for each ω. From the simulations it is clear that a wide variety of tilt angles apart from those close to zone axes show images that could be interpreted as structural images. Lattice fringes (one-dimensional resolution) appear to be present in images tilted several degrees away from the lattice planes (fig. 4). The planes present in such images does not reflect the interplanar distances in the particle meaning that caution has to be taken when deducing anything about atomic distances or e.g. surface relaxation in small metal particles directly from micrographs. If the projected direction is not definitely determined, measuring interplanar spacings can give severe errors. A line scan perpendicular to the apparent planes in fig. 4 shows that the distances between the planes varies ≈10% within the image. In the tilt series it is also possible to find false two-dimensional resolution that erroneously could be interpreted as e.g. the particle being projected along the $<110>_{ccp}$ direction (e.g. fig. 5). The difficulties in properly interpreting the projected direction is enhanced when the particles are imaged supported on amorphous substrate.

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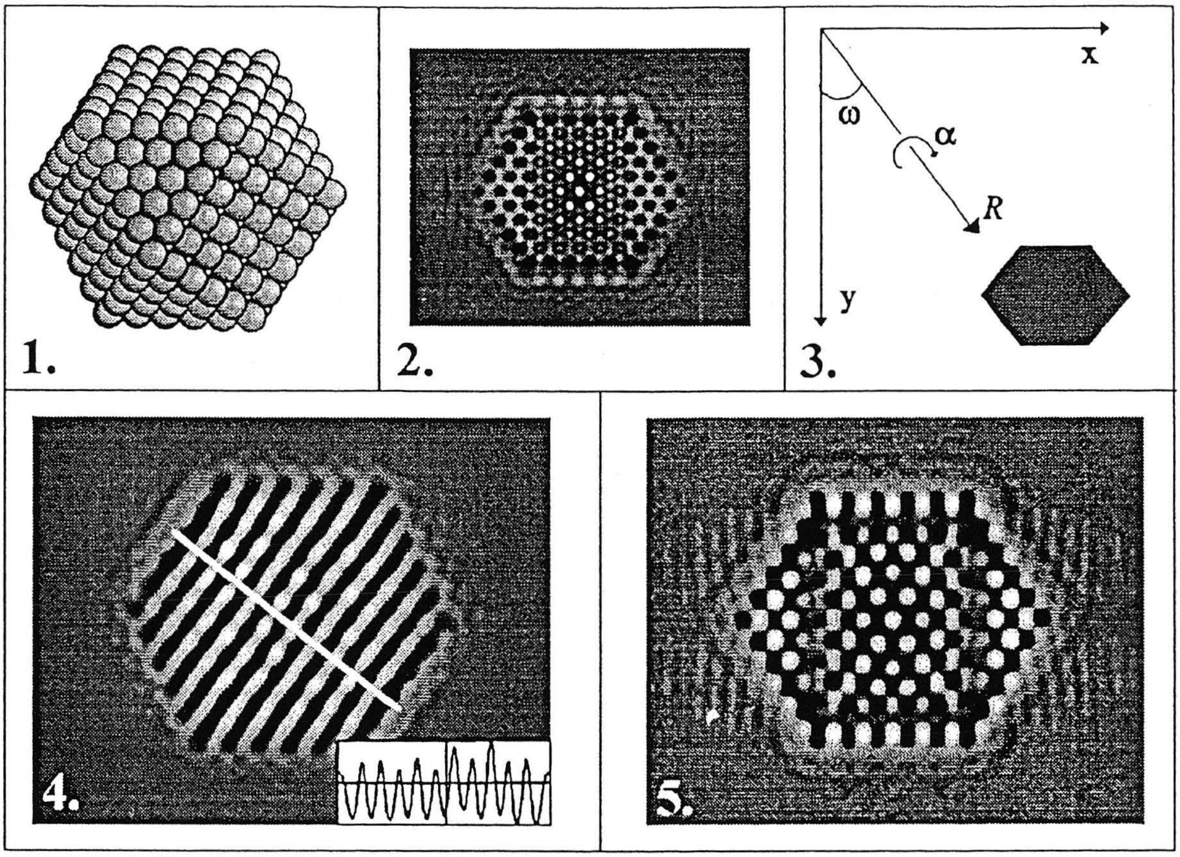

Fig. 1: Model of a five shell cubeoctahedron. This is the atomic structure of the particle used in the simulations.
Fig. 2: Simulated image of a palladium particle viewed along the <111>$_{ccp}$ direction
Fig. 3: Coordination system defining the projected direction of the particle. The schematic cubeoctahedron shows the initial position of the particle. The direction of the rotation axis, *R*, is determined by the angle ω and the rotation around this axis is given by the angle α.
Fig. 4: Simulation of a particle tilted 20 degrees around a rotation axis with ω=63 degrees. Analyzing the minima from a line scan along the white line it can be shown that the apparent interplanar distances varies ≈10% within the particle.
Fig. 5: This particle has been tilted 15 degrees with ω=0. Situated on an amorphous substrate this particle could misinterpreted as showing structural resolution.

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Laserprinter printouts of the full simulation series can be obtained from Jan-Olle Malm (address above).