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HRTEM and HAADF Analysis of Ni Multi-Twinned Nanoparticles

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Metal nanoparticles (NP) are being extensively studied because of their unique properties with respect to bulk materials, and consequently because of their technological applications in various areas. For instance, magnetic NP show very interesting potentiality in development of high density memories and in selected application of medicine, like biodetection, targeted drug delivery, and magnetic fluid hyperthermia.

In this work, we report our results of a study of Ni NP. Ni NPs have received less attention with respect to other magnetic NPs [1] and less is known about their structural properties. In our experiment Ni is evaporated by magnetron sputtering, and it is condensed into NP by an inert gas carrier (in our case, Ar). In our setup the charged NP in the produced beam are mass selected by an electric quadrupole and enter in the deposition chamber where they are deposited on a substrate.

We studied the nanoparticles crystalline structure by HRTEM and HAADF in a JEOL JEM-2200 FS with Objective lens spherical aberration Cs=0.5 mm and operated at 200 KeV.

The HRTEM analysis in fig 1a shows the typical contrast features of mutitwinned icosahedric NP (MTNP) that so far has not been reported, to author's knowledge, for any Ni NP.

To confirm this assessment simulations have been performed based on STEM_CELL package for (S)TEM simulation[2], the input was an unrelaxed atomistic model based on Mackay construction for the icosahedral structure [3].The use of this model is justified by the observation on other materials with similar structure that this does not affect the main contrast features [1].

A direct comparison of HRTEM (fig 1 a) with multislice (fig 1b) demonstrates that the experimental contrast can be completely explained in term of the MTNP. This was also confirmed by the analysis of atomic resolution HAADF images compared with kinematical HAADF simulations (fig 1 c,d) [4]. These simulation permit to qualitatively explain the larger intensity in the center of the particle even without considering channeling effects.

A very good agreement is obtained in both cases considering the MTNP. The fringe contrast in the NP has been also systematically studied and successfully compared in other high symmetry directions of the icosahedron.

We studied in particular the possible formation of defects and irregularities. The delocalization of lattice fringes in HRTEM may play an important role and we compared all results with simulations. For a more precise comparison the experimental amorphous diffractogram has been manually fitted to estimate defocus and convergence (see inset of fig 2a).

Fig 2a shows in facts, in correspondence with the arrow, an apparent dislocation. Simulations with the correct defocus show that this effect is due to the fringe superposition of parts of the structures with different orientations. Conversely fig 2b shows a small NP with an evident left-right asymmetry which cannot be explained by any simulation and could be possibly indicative of a misalighned twinning plane in the two part of the NP.

Finally we evaluated in fig 2c the lattice deformation using GPA [4] in the "radial direction" and found a monotonic increase of the lattice parameter as in the case of FePt [1]. The evaluation based on the simulation with unrelaxed structures with the same imaging parameters produced a similar but much lower deformation.

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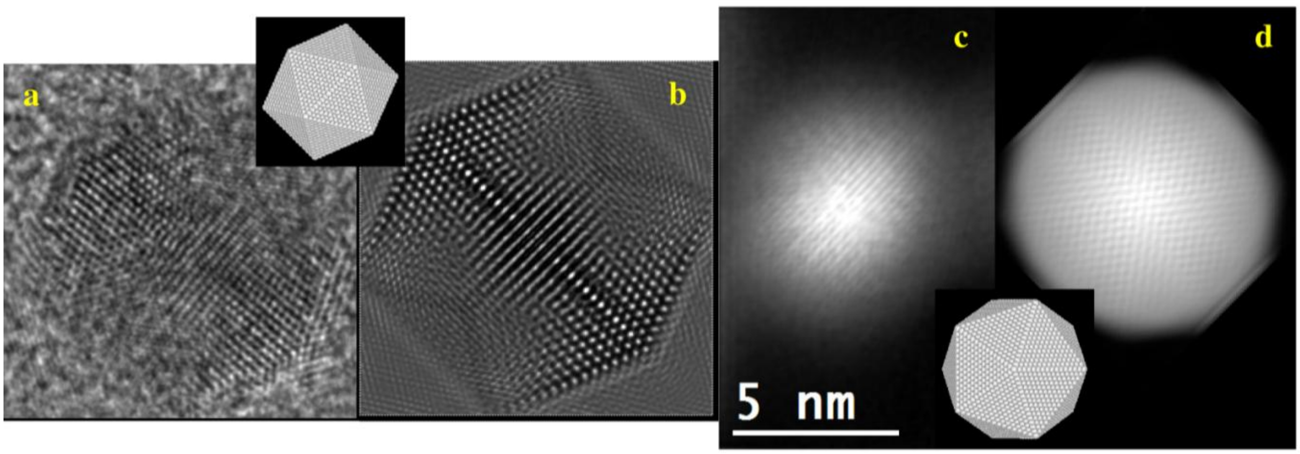

FIG. 1. HRTEM (a) and relative simulation (b) of a Ni NP the NP orientation is indicated in the inset. Fig c,d show an atomic resolution HAADF image and relevant simulation in another direction indicated by the model in the inset

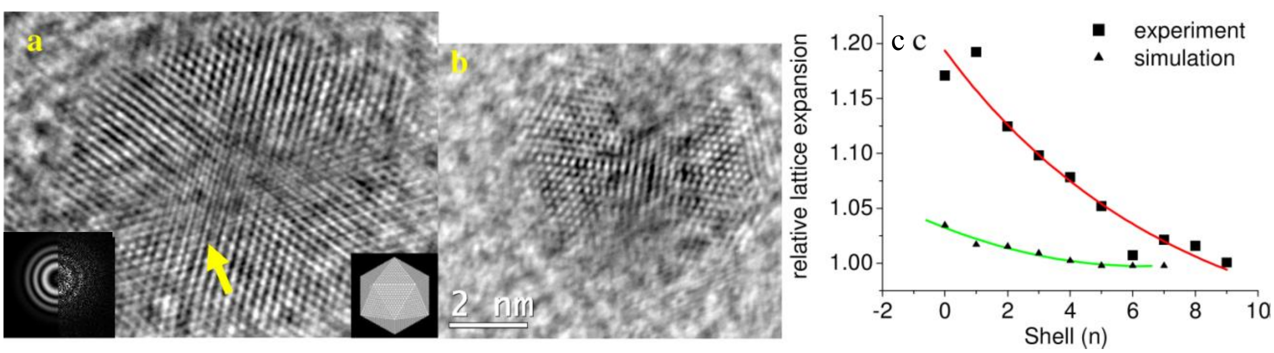

FIG. 1. A) HRTEM picture of a particle in a different orientation (indicated by the model in the right inset). The left inset shows the diffractogram fitting (defocus=-95nm convergence 0.4mrad). The arrow indicate an apparent dislocation due to atomic fringes superposition. b) small nanoparticles with evident asymmetries c) deformation of the radial (111) fringes as a function of the shell (0 is the outer). Triangles refer to simulations while squares to experiments.

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