Twinning Evolution of Faceted Face-Centered Cubic Fe Nanoparticles under Electron Irradiation

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Metal nanoparticles have attracted extensive attention for their potential applications in catalysis, photonics, plasmonics, and information storage. In-situ high-resolution transmission electron microscopy (HRTEM) is becoming an important tool to understanding the nucleation and growth mechanism by observing structural fluctuations of the metal nanoparticles at atomic scale in real time.

Twinning of nanoscaled particles is common feature and widespread in face-centered cubic (FCC) metals, such as Ag, Au, and Cu. By traditional synthetic methods, such as thermal decomposition and chemical reduction, Fe nanoparticles with body-centered cubic (BCC) structure are usually expected. In our previous work, we have successfully synthesized icosahedral, decahedral, and fivefold twinning Fe nanoparticles with FCC structure by a thermodynamic controlled method [1,2]. Here, we report the in-situ HRTEM observation of the twin evolution process in FCC Fe nanoparticles under electron irradiation. The twinning mechanism could be a nucleation and growth mechanism for FCC materials, and it could also be utilized to tailor the surface structure and surface chemistry of nanoparticles.

In-situ HRTEM observations were performed by using a FEI Titan 80-300 imaging spherical aberration (Cs) corrected microscope operated at 300 kV. In the experiment, the Cs value was carefully adjusted to a range of -2~3 μm. Images were taken near in-focus. Under these specific experimental conditions, as shown in Figure 1, the {111} and {220} lattice plane distances of fcc-Fe which are 0.206 and 0.126 nm, respectively, can be clearly observed.

Figure 2 is a sequence of HRTEM images of twin growth between two FCC Fe nanoparticles. Figure 2(a) was taken at overfocus, in which atomic sites appear bright on a dark contrast. 10 seconds later under electron irradiation, Figure 2(b) was acquired at underfocus, in which contrast was reversed into dark on bright. Initially, these two particles were close enough and engaged each other with a small misorientation along the electron beam direction. Under electron beam irradiation, the particle on top left grew up by the propagation of twins towards the particle on bottom right. The thickness of the growth twin increased from 3 to 5 atomic layers [from Figure 2(a) to Figure 2(b)]. 1/6[112] twinning dislocations (indicated by arrow) were observed to emit from left surface facet, and end at the right surface, as shown in Figure 2. The twinning mechanism is illustrated in Figure 3.

References

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**FIG. 1.** Contrast transfer function of the 300-kV FEI Titan 80-300 Cs corrected TEM with which the HRTEM images were taken. Under these experimental conditions, spatial frequencies in the band between 4.85 and 7.94 nm$^{-1}$ representing FCC Fe (111) and (220) plane distances of 0.206 and 0.126 nm are transferred with the same contrast.

**FIG. 2.** HRTEM image sequence of FCC Fe nanoparticles, showing growth of twin through dislocation mechanism; see text for details.

**FIG. 3.** A schematic of the twin propagation and the emission of the dislocations from left to right surface. SISF: superlattice intrinsic stacking fault; SESF: superlattice extrinsic stacking fault.