Electronic Supplementary Material (ESI) for CrystEngComm

Growth defects and epitaxy in Fe_3O_4 and γ-Fe_2O_3 nanocrystals

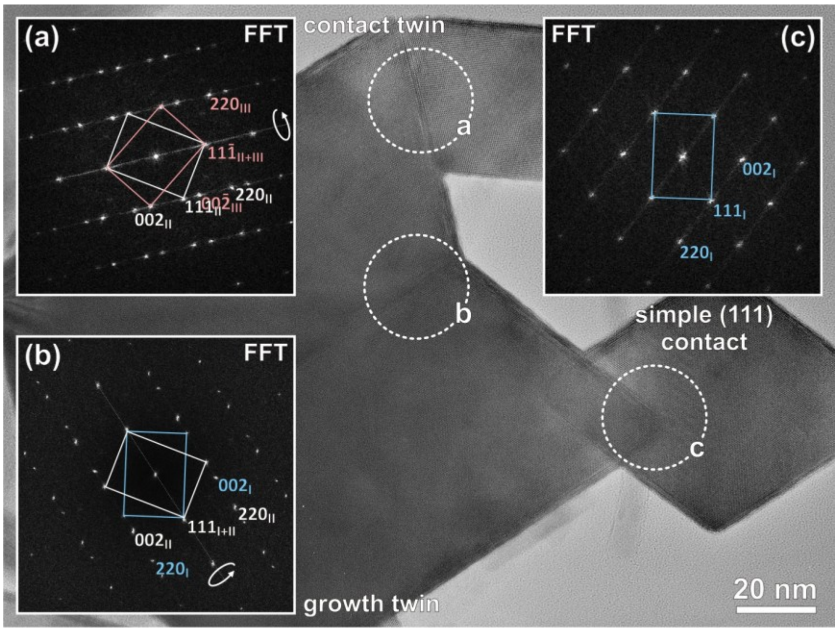
Aleksander Rečnik,[a] Ilona Nyirő-Kósa,[b] István Dódony [c] and Mihály Pósfai [b]*

[a] Department for Nanostructured Materials, Jožef Stefan Institute, Ljubljana, Slovenia
[b] Department of Earth and Environmental Sciences, University of Pannonia, Veszprém, Hungary
[c] Department of Mineralogy, Eötvös L. University, Budapest, Hungary

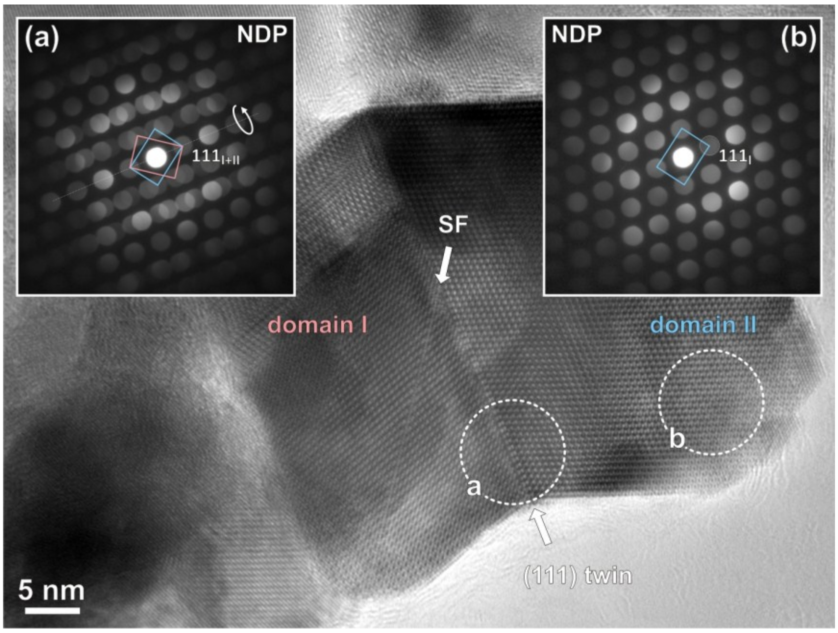
(cover page)

Supplementary Information

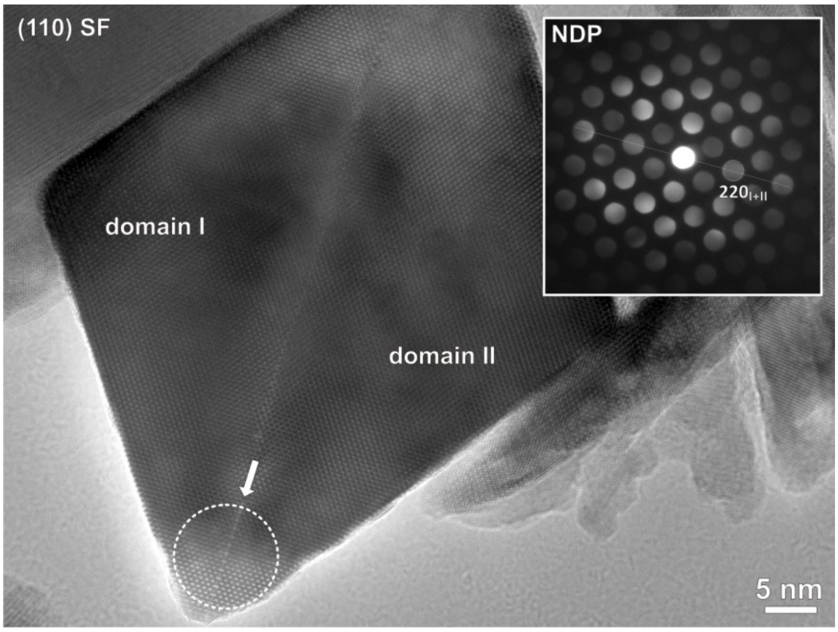
The following materials provide additional crystallographic information on orientation relationships of observed twin boundaries, stacking faults and epitaxial layers in magnetite and maghemite nanocrystals, based on FFT analysis and nano-diffraction data.



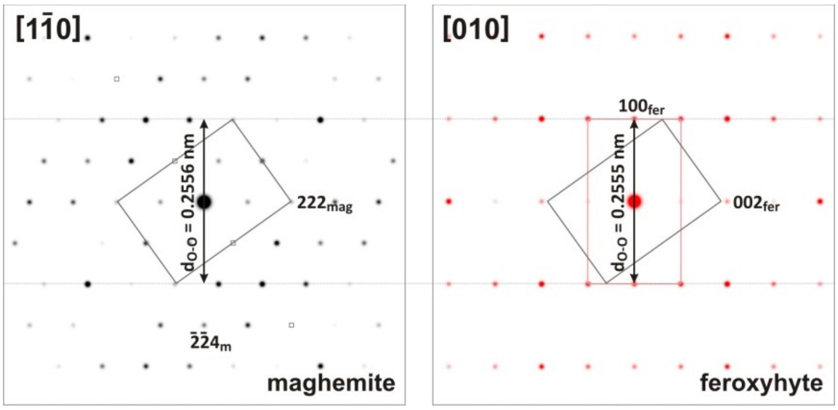
Supplemental Figure S1: FFT analysis of crystal orientations from Fig. 2a. Reciprocal space images confirm that the interfaces marked (**a**) and (**b**) are 180° twin boundaries, whereas the crystal in (**c**) is in identical orientation as the hosting crystal. Diffraction data shows no difference between the growth and contact (111) twin.



Supplemental Figure S2: Diffraction analysis of maghemite nanocrystal from Fig. 3a containing twin boundary and a stacking fault (SF). Experimental nano-diffraction patterns (NDP) from two areas: (**a**) twin boundary and (**b**) single crystal domain II. In semi-kinematic scattering regime, relative intensities of diffraction disks in thin crystals are proportional to structure factors of individual reflections. Nano-diffraction pattern from the (111) twin boundary is a combination of reflections from both domains (**I+II**). SF is analyzed in the following Figure.



Supplemental Figure S3: Diffraction study of stacking fault (SF) in maghemite crystal shown in close-up in Fig. 3b. Nano-diffraction pattern (NDP) shown in the inset was recorded in the thin crystal region containing the SF. Both crystal domains (**I**+**II**) are in identical orientation across the SF running along the (110) plane of the spinel structure. NDP displays no splitting of the diffraction disks, indicating a simple lattice translation across the SF, whereas their relative intensities correspond to a single crystal of spinel.



Supplemental Figure S4: Comparison of maghemite and feroxyhyte diffraction patterns in the orientation relationship as observed on the maghemite-feroxyhyte epitaxial layers, shown in Fig. 4, where (002) planes of feroxyhyte are grown epitaxially on {222} planes of maghemite. The two lattices have different d-spacings in the direction normal to the interface, whereas their in-plane matching is almost perfect because of the very similar O-O distances. Other Fe-oxides and hydroxides, listed in Table I, have worse match with maghemite.