HRTEM observation of the monoclinic-to-tetragonal (*m*-*t*) phase transition in nanocrystalline ZrO_2

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Monoclinic-to-tetragonal ($m \rightarrow t$) phase transitions within unconstrained nanoparticles of ZrO_2 *in situ* observed and characterized with high-resolution transmission electron microscopy (HRTEM) lead to the following orientation relations between the phases: 1) *m*(100) || *t*(110), *m*[001] || *t*[001]; 2) *m*(013) || *t*(116), *m*[001] || *t*[001]; 3) *m*(100) || *t*(001), *m*[001] || *t*[110]; 4) *m*(011) || *t*(100), *m*[001] || *t*[110]. The relations 1and 3 occur most frequently; the relations 2 and 4 were found only in combination with 1and 3 in the "core-shell" structures. The tetragonal phase nucleates at the free (100) surfaces of the monoclinic particles. During the transition both the phases coexist within a particle; the *m*-*t* interface is coherent. A geometric model of the interface is proposed.

The transition is induced by the electron beam and occurs within the region of thermodynamic instability of the bulk tetragonal phase of zirconia. The tetragonal phase is stabilized by small crystallite size due to the lower surface free energy of *t*-ZrO_2.