Detection of vacancies in FCC solid and their effect on twinning

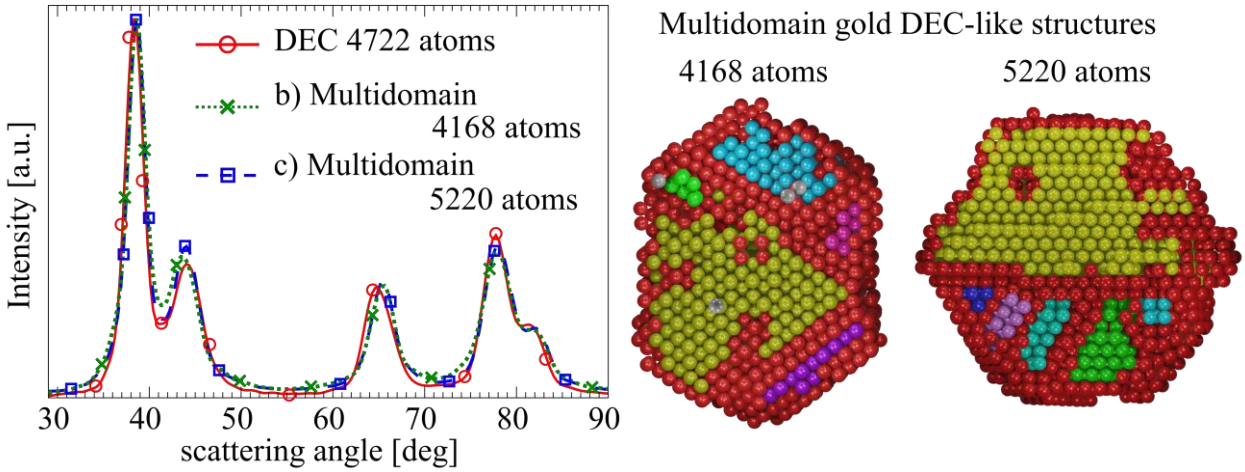
Ilia Smirnov [a], Zbigniev Kaszkur [a], Armin Hoell [b]

[a] Institute of Physical Chemistry, Warsaw, Poland

[b] Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

TEM observations reveal FCC nanoparticles (NPs) in different morphologies: cuboctahedron (CUB), decahedral (DEC), icosahedral (ICO) or their imperfect variations. The two latter perfect morphologies are special cases of stable multitwinned structures. The twinning occurs relative to (111) planes when fcc ABCA sequences during quick atom deposition turn locally to ABAC forming mirror B plane with lattice energy barely changed. Having eight [111] directions the cross-twinning may occur forming complex multitwinned NPs. However, the exact mechanism that initiate these processes is unknown.

We developed a computational approach to simulate the twinning: large number of atoms is deleted from regular CUB model and energy relaxed. This leads to multitwinned NP with XRD pattern similar to DEC.



Combined synchrotron in-situ SAXS and WAXS techniques (Hamburg, Petra III, beamline P62) were applied to prove the role of vacancies. Gold NPs (average size ~2.3 nm) were irradiated with X-ray beams. Depending on the X-ray flux intensities, two types of NP evolution were found:

- ***for low-flux***: WAXS & SAXS analysis shows NPs growth and decrease of NPs density. These observation can be interpreted as an **accumulation of vacancies** inside NPs.

- ***for high-flux:*** WAXS & SAXS analysis shows decrease of NP size and rise of NPs density. These observation can be interpreted as a quick **accumulation** followed by vacancies **healing**.

These indirect observations of vacancies proves their role in evolution of NPs morphology.