Role of pre-existing dislocation in Pt nanoparticle submitted to uniaxial compression

Julien Godet[1*], Laurent Pizzagalli[1], Marie-Ingrid Richard[2], Stéphane Labat[3]

[1]Institut Pprime – Poitiers, [2]CEA-IRIG, [3]IM2NP – Marseille

*julien.godet@univ-poitiers.fr

Résumé pour : oral

Defects in crystals, whether 2D (e.g., grain boundaries and stacking faults), 1D (e.g., dislocations), or 0D (e.g., point defects), have a critical influence on the properties of bulk solids. At the nanoscale, a single defect can completely alter the properties of a nanocrystal. Furthermore, due to the proximity of surfaces, the energy and mobility of defects in single nanostructures differ greatly from those in bulk materials. Crystal defects are not the sole determinants of mechanical behavior. In fact, it has been recognized that defects of various natures and length scales are not necessarily adverse, but can instead give rise to specific functionalities, such as improving adsorption affinity or catalytic activity. This defect sensitivity could lead to new approaches for engineering the properties of nanostructures by introducing specific defects. To do so, we must first understand the behavior of defects (nucleation, movement, annihilation, and interaction between defects) and the strain fields surrounding them in nanostructures under external loads.

Thanks to the high brilliance, coherence, and flux of synchrotron X-ray beams, Bragg Coherent Diffraction Imaging (BCDI) can image single defects in nanocrystals in three dimensions, together with the displacement field and, in particular, their interactions with surfaces in nanoparticles. In this study, we examined a platinum nanoparticle (NP) deposited on sapphire that contained a pre-existing dislocation. To investigate the stability of the defect, we used molecular dynamics simulations on the NP containing the dislocation. We extracted the shape and defect geometry from the BCDI images. First, we studied the defect's stability, then we subjected it to uniaxial compression to understand the role of the pre-existing dislocation inside the nanoparticle.

Through this study, we will demonstrate how to create a realistic numerical sample based on experimental data and discuss the stability of the dislocation and its contribution to plasticity when the NP undergoes external loading.

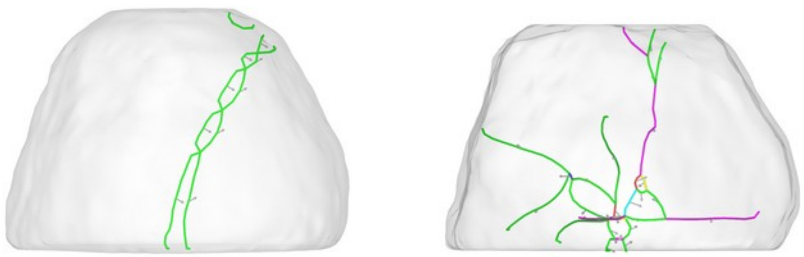

Figure : (left) dissociated dislocation introduced in Pt NP with a diameter of 20 nm. (Right) microstructure after a uniaxial compression of 8.6%.

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