Role of the twin boundary junctions in the initial deformation mechanisms of nanotwinned thin films: insights from atomic-scale simulations

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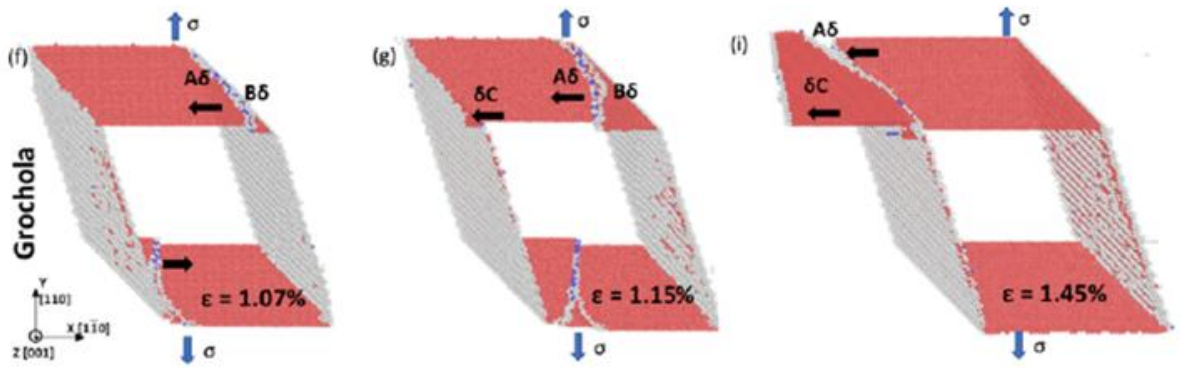
Nanotwinned (NT) face-centred cubic metals are of significant interest due to their exceptional ability to combine both strength, ductility and electrical resistivity [1]. Twins are delimited by {111} coherent twin boundaries (CTBs) that are close and parallel to each other and, very often, by {112} symmetric incoherent twin boundaries (ITBs) [2]. We studied with molecular dynamics simulations the behaviour of the CTB-ITB junctions, to determine their role in the initial deformation mechanisms of nanotwinned gold thin films.

To focus on the role of the CTB-ITB junctions, the studied structure consists of a single twin delimited by two CTBs and two ITBs. As already observed in previous studies, the initial deformation mechanisms show detwinning and migration of the CTBs. However, for the first time, we put in evidence reactions between the dislocations issued from the two dislocation sources that are the ITBs.

Moreover, we recently published experimental results on tensile tests of gold single crystals containing nanometric isolated twins [3], i.e. with structures similar to the simulated samples. The present molecular dynamics simulations allow a better characterization of several plasticity mechanisms observed experimentally with transmission electron microscopy.

[1] L. Lu et al, *Science* 304 (2004) 422–426; L. Lu et al, *Science* 323 (2009) 607–610
[2] L. Liu et al, *Phys. Rev. Lett.* 106 (2011) 175504; D. Bufford et al. *Acta Mater.* 59 (2011) 93–101
[3] P. Godard et al, *Phys. Rev. Mat.* 9 (2025) 103602



Three steps of the deformation of a nanotwin (the CTBs are in red, the ITBs in white and atoms in an FCC environment are not represented). As in in situ transmission electron microscopy experiments [3], glide of twin dislocations and emission of dissociated perfect dislocations are observed.