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[1] Seo, J.-H. et al., Nano Letters, 2011, 11, 3499-3502 [2] Dao, M. et al., Acta Materialia, 2006, 54, 5421-5432

NUMERICAL SIMULATIONS OF TWIN FORMATION AND EXTENSION IN FACE-CENTERED CUBIC METALLIC FILMS

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The basic mechanisms of plasticity in face-centred cubic materials are now well known in bulk materials. However, several experimental studies have shown that at the nanoscale, some of its mechanisms can induce surprising mechanical properties when compared to bulk behaviour. The formation and extension of twins in metallic nanowire can, for example, generate super-plasticity [1] or the presence of growth nano-twins within a material can lead to strengthening effects [2]. Atomic simulations are particularly adapted for studying the plasticity mechanisms at play, since they allow their visualization at the atomic scale.
While many atomistic simulations studies have been focused on the interaction of dislocation with a twin boundary, our study differs in the choice of crystallographic orientations, specifically designed to facilitate twin formation. In that context, we analyse, in a thin face-centred cubic metallic film, the competition between free surfaces and twin boundaries for twin nucleation under applied stress, as well as the influence of a pre-existing twin boundary on the newly nucleated twin propagation. The chosen orientation also allows the introduction of surface defects, namely monoatomic surface steps, which can act as dislocation sources under mechanical stress.
Our study highlights the influence of these surface defects on plasticity, by the comparison of systems with and without surface defects. In particular, the presence of a surface step on the surface localizes the plasticity, which gives rise to specific reactions in the presence of a pre-existing twin boundary, causing the formation of a Lomer dislocation, and subsequently the formation of a Lomer-Cottrell lock. When no defect is present at the surface, we observed the nucleation of several nano-twins, generating a partial reorientation of the film and the partial suppression of the original twin boundary.

References
[1] Seo, J.-H. et al., Nano Letters, 2011, **11**, 3499-3502
[2] Dao, M. et al., Acta Materialia, 2006, **54**, 5421-5432