

Plastic deformation in nano-objects: stress localization and geometry

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Résumé pour : poster

The plastic deformation of crystalline nanostructures is often driven by mechanisms involving the heterogeneous nucleation of dislocations, mainly because these systems are characterized (i) by a large surface-volume ratio, (ii) a low density of initial defects and a limited available volume which hinder usual bulk plasticity mechanisms. In nanoparticles under compression, the nucleation of dislocations occurs in near-surface regions where stresses concentration can be observed due to the contact with the indenter. Theoretical investigations showed that the stress magnitude and localization depend on the geometry of these regions, which may explain the shape dependence of nano-objects mechanical properties [1]. Despite significant theoretical efforts, this property remains far to be fully characterized and understood. Furthermore, the respective influences of nano-objects shape and dimensions on dislocation nucleation are yet to be discriminated and quantified.

In this study, we investigate the influence of shape and size of nanocrystals on the relation between the applied stress and the resulting local stress concentration, by performing 2D and 3D molecular dynamics compression simulations [2]. Our results allow for elucidating how dimensions and surface contact angle could modify the stress concentration, and therefore the onset of plasticity in the nanocrystals. We find that a simplified analysis based on elasticity theory fails at fully explaining our results. In fact, it is necessary to take into account the influence of surface stress. Another issue is the difficulty to rigorously determine a critical exponent for the stress variation. In this contribution we propose an alternative model based on the elastic interaction between the different stress concentration regions in the nanocrystals [2].

[1] J. Amodeo, L. Pizzagalli, *Comptes Rendus. Physique*, 22 (2021) no. S3, pp. 35-66.

[2] L. Pizzagalli et al., *J. Mech. Phys. Solids* 205 (2025) p 106306