

Thematic Session (eg. Nanophotonics & nano-optics, nanomaterials, nanobioscience ...):

Nanomechanics: surface/ interface, composite nanomaterials, hybrid nanomaterials

Keywords (max. 4-5): **core-shell nanoparticle, nanocompression, SEM, molecular dynamics, dislocations**

Disciplinary fields involved (eg. Chemistry, Physics, Biology ...): **Mechanics, physics**

Sustainable Development Goals* eventually involved in your research: 9

When more is less: the effect of grain boundaries on the mechanical properties of metal nanoparticles

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We present recent experimental and numerical data on the compression behavior of single crystalline and core-shell metal nanoparticles. Single crystalline samples deform elastically up to very high level of stresses approaching the theoretical shear strength. The following catastrophic plastic collapse is characterized by multiple dislocation nucleation events in the pristine nanoparticles. In the experiment, depositing an ultrathin (15 nm) nanocrystalline overlayer of Au on single crystalline Ag particles of hundreds of nanometers in diameter changes their deformation mode from that characteristic of single crystalline nanoparticles (high strength, wild strain burst) to a lower flow stress and strain hardening regime. Thus, paradoxically, adding more load-bearing material to the particles by coating them with a nanopolycrystalline phase drastically decreases their strength. This behavior is confirmed by molecular dynamics nanocompression simulations. Indeed, the mechanics of single crystalline core – polycrystalline shell Ag-Au nanoparticles under compression is investigated and compared to single crystalline samples. The results confirm the important role played by the dislocations nucleation process in the nanocrystalline shell (prior to the crystalline core) in which the large amount of grain boundaries promotes strain hardening.