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[1] Y. Mishin, D. Farkas, M. J. Mehl, and D. A. Papaconstantopoulos : Interatomic potentials for monoatomic metals from experimental data and ab initio calculations. Phys. Rev. B 59, 3393 – Published 1 February 1999. [2] Y. Mishin, M. J. Mehl, D. A. Papaconstantopoulos, A. F. Voter, and J. D. Kress : Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations. Phys. Rev. B 63, 224106 – Published 21 May 2001.

Mechanical response of face-centered cubic metallic nanospheres under uniaxial compression

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Context

Nano-objects often exhibit drastically different properties compared to their bulk counterpart, opening avenues for new applications in many fields, among which advanced composite materials, nanomanufacturing, or nano-electromechanical systems. For instance, it has been recently shown that nanowires exhibit enhanced mechanical properties. The literature regarding the plastic deformation of a single nanoparticle is more recent and more limited. In this study, we have performed molecular dynamics simulations to investigate the mechanical behavior of metallic nanoparticles.

Objectives :

⇒ Study the size effects on mechanical properties of nanoparticles.

⇒ Modelling of the plasticity of "ideal" single metallic nanoparticles :
↳ Dislocation nucleation.
↳ Propagation of dislocations in the nanoparticle,
↳ Release of dislocations...

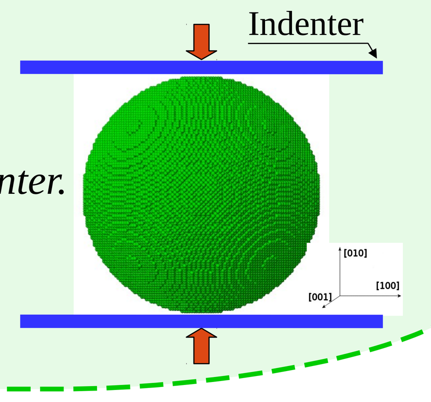
Method

Classical molecular dynamic simulations are performed using the code LAMMPS [1], developped by Sandia National Laboratories, using a time step of 0.001 ps. The embedded atom method (EAM) potential function (parameterized by Mishin et al.[2]) is used to describe the interactions between aluminum atoms with a lattice constant of 4.05 Å. A Nose-Hoover [3] thermostat was applied to thermally equilibrate the system at 10 K. The system was compressed along the [010] crystal direction with a velocity of 10 m.s^{-1}, corresponding to a strain rate of 10^{9} s^{-1}.

Two planar indentation potentials were used to compress the sphere, one placed above the sphere and the other below. This potential applies a force onto atoms according to their coordinates as given by :

$$F_y(y)=k(y-y_i)^2$$

↳ F_y : *The force in the [010] direction applied on atom i by the indenter*
↳ k : *A constant (taken to be 1000 eV/A) related to the effective stiffness of the indenter.*
↳ y_i : *Position of atom i along [010].*
↳ y : *Position of the indenter along [010].*



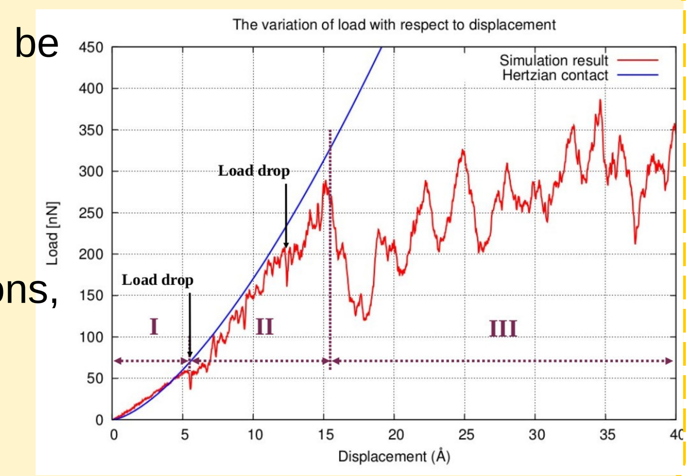
Global behavior

For spherical nanoparticles, the deformation process can be divided into three steps:

(I) Elastic deformation,

(II) Hillock formation by nucleation and migration of dislocations,

(III) Nucleation of dislocations from the hillock structure.



Elasticity (I)

Three forms of nanoparticles were used to study the size effect on the mechanical behavior.

Cube | Cylinder (height=diameter) | Sphere

Forme	Cube			Cylinder (height=diameter)			Sphere		
Edge or Diameter (nm)	4.83	9.68	16.1	5.25	10.5	17.5	6	11.74	20
Number of atoms	6912	55296	256000	7145	56215	255647	7011	50861	252425
Elasticity modulus (GPa)	40.2	56.6	63.2	48.7	52.7	63.2	95.9	158.1	114.23

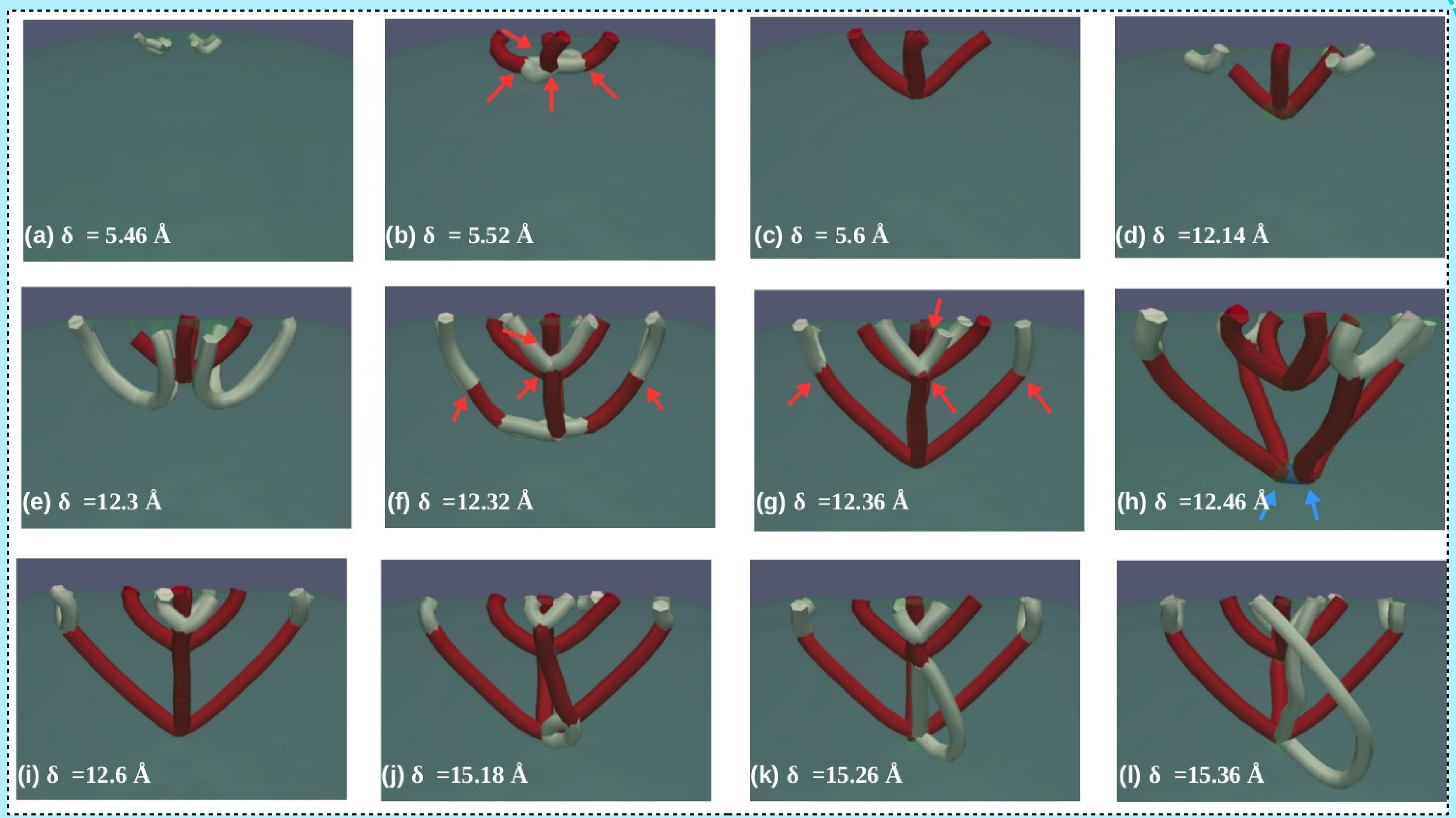
- The elastic moduli of nano-objects are different from the one of the bulk counterpart (The bulk value is worth equal to 63 GPa), and exhibit a size dependence.
- In the case of cubic and cylinder nano-objects, the elastic moduli increase with the size. However, for the largest investigated sizes, the elastic moduli converge to their bulk value.
- In the case of spherical nanoparticle, the values of moduli obtained by applying the classical Hertzian theory [4] predicts the relationship between applied load F and compression depth δ as :

$$F=\frac{4}{3}E_r R^{1/2}(\delta/2)^{3/2}$$

With E_r is the reduced Young's modulus of the sphere.
- This moduli does not depend only on the size of nanoparticle but also of contact surface, which evolves itself non linearly with the diameter of the nanoparticle. During further compression, the nucleation of dislocation events are accompanied with a drop of the load [5].

Plasticity (spherical nanoparticles)

- **Hillock formation by nucleation and migration of dislocations (II)**



Visualization of the evolution of dislocation structures during plastic deformation (Visualization using ParaView): white line, shocley partial dislocation with Burgers vectors 1/6 <112>; red line, stair-rod dislocation with Burgers vectors 1/3 <100> and blue line, stair-rod dislocation with Burgers vectors 1/3 <110>.

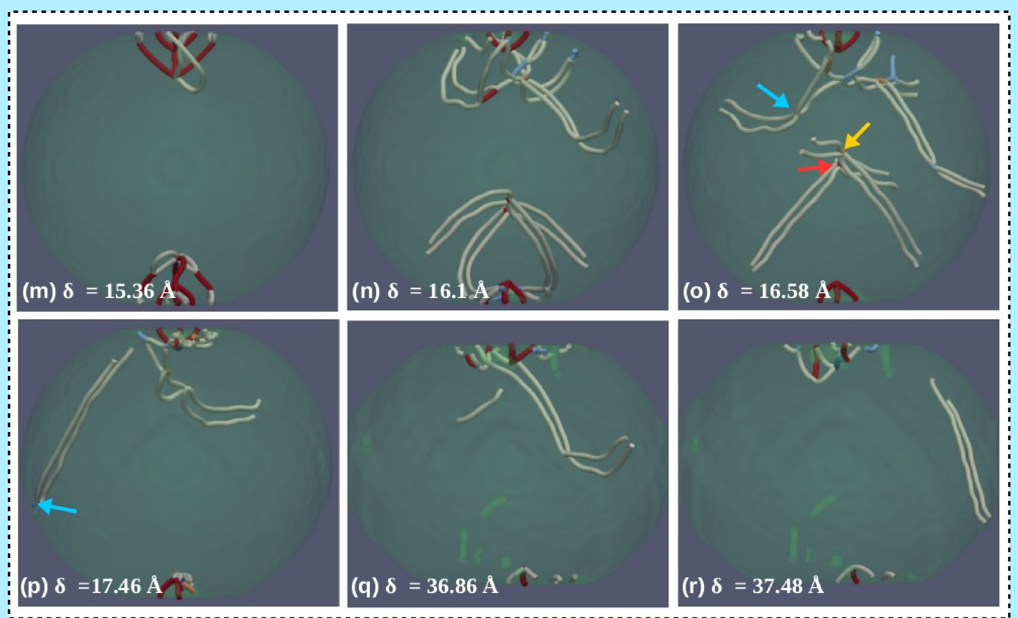
(a) Nucleation of Shockley partial dislocations from the contact edge.
(b+c) The intersection of Shockley partial dislocations on four {111} planes, as marked by red arrow, form a four stair-rod partial dislocations 1/3 [100] and a pyramid hillock structure. Such dislocation reaction is given by: $\frac{1}{6}[11\bar{2}]+\frac{1}{6}[1\bar{1}2]\rightarrow\frac{1}{3}[100]$

(d) The hillock acts as a stress concentrator to activate dislocation nucleations. Nucleation of Shockley partial dislocations from the edge of the second atomic layer (the first atomic layer is totally flattened).
(e+f+g) These partial dislocations propagate and intersect, as marked by red arrows, to form a second pyramid sessile structure.
(h) The intersection between two stair-rod dislocations, as marked by blue arrow, can also form another stair-rod dislocation 1/3 [-101]. Such dislocation reaction is given by:

$$\frac{1}{3}[\bar{1}00]+\frac{1}{3}[001]\rightarrow\frac{1}{3}[\bar{1}01]$$

(i) The second pyramid is formed.
(j+k) A stair-rod dislocation dissociates into two Shockley partial dislocations.
(l) This partial dislocation, with one end starting at the surface and another end pinning at the tip of outer pyramid hillock, grow from the edges of the pyramid hillock.

- **Nucleation of dislocations from the hillock structure (III)**



Visualization of the evolution of dislocation structures during plastic deformation (Visualization using ParaView): white line, Shocley partial dislocation with Burgers vectors 1/6 [112]; red line, stair-rod dislocation with Burgers vectors 1/3 [100]; orange line, stair-rod dislocation with Burgers vectors 1/6 [1-10]; blue sky, perfect dislocation with Burgers vectors 1/2 [110].

(m+n) Dislocations are released from the tip of the outer pyramid hillock and glide into the nanosphere.

(o+p) Moving dislocations may meet and interact, forming another type of stair-rod dilocations (interactions indicated by red arrows).

(q+r) Free dislocations glide to the opposite side of the surface and escape from the nanoparticle.

Acknowledgements:
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