PhD topic

Study of plastic deformation by diffusion at the nanometer scale

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Team	PDP		
Keywords	Nanoparticles	Diffusion	Metals
	Numerical simulations	Plasticity	

Subject description

When the characteristic dimensions of materials decrease to nanometric scales, their properties become increasingly dependent on surfaces and less and less on volumes. For example, nano-objects such as nanowires or nanoparticles are highly resistant to deformation because there are few, if any, defects already present in the volume that could facilitate plasticity. Experiments and simulations show that it is necessary to create new defects from the surfaces, which requires very high applied stresses.
Recent experiments have shown that below a certain size, another mode of plastic deformation can be activated under stress, in which atomic diffusion at the surface of the nano-object (or at the interface with the system applying the stress) plays a central role [1]. Under these conditions, the nano-object, which is usually metallic, appears to behave like a liquid, with diffusion of the material allowing the stresses to relax. This mode has not yet been studied in depth and remains somewhat mysterious. A major obstacle is that it occurs at dimensions smaller than ten nanometers, which makes experiments difficult. Another problem is that it is a diffusive mechanism, which makes it difficult to model using techniques such as molecular dynamics.

Here, we propose to study this mode of deformation using various approaches that are more suited to modeling diffusion mechanisms. Initially, we will focus on the ART-nouveau method. This method allows rapid exploration of the energy landscape by searching for transition states. Diffusion events can therefore be systematically determined for surface atoms in the presence of an applied constraint. A first objective will be to test the use of the ART-nouveau method for this problem and to develop tools to automate the search for transition states and data exploitation. Kinetic Monte Carlo (KMC) calculations can then be performed using this database to determine the diffusion dynamics at a given temperature. Repeating this procedure for various applied stresses and sizes will also make it possible to identify the conditions (dimensions, temperatures) favorable to this mode of deformation.

Depending on the progress of the work, we plan to implement other numerical techniques (atomic Monte Carlo, Parallel Replica Dynamics, Temperature Accelerated Dynamics) suited to the study of diffusion mechanisms.
During the thesis, we will focus on face-centered cubic metal nanoparticles, modeled using EAM potentials, whose plasticity mode through dislocation nucleation is already known [2].

[1] Ding et al, Acta Materialia **293**, 121092 (2025)
[2] L. Pizzagalli et al, Scripta Materialia 241, 115863 (2024)

Candidate profile

The thesis is based exclusively on performing numerical simulations on a computer in a Linux environment. To achieve the objectives, you will need to use a variety of digital tools and handle large amounts of data. This will require writing short Python code snippets. You must therefore be comfortable with computers and not averse to programming in general. Scientific curiosity, analytical, synthesis, and communication skills are also desirable.

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