PhD proposal

Plastic deformation by diffusion at nanometric scales

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

We propose to study this mode of deformation using an ART-nouveau approach. This allows rapid exploration of the energy landscape by searching for transition states. Diffusion events can thus be systematically determined for surface atoms, in the presence of applied stress. The initial focus will be on an aluminum nanoparticle modeled by an EAM potential, whose plasticity mode by dislocation nucleation is already known [2]. A first objective will be to test the use of the ART-nouveau method for this problem, and to develop tools to automate transition state searches and data exploitation. In a second phase, kinetic Monte Carlo (KMC) calculations can then be carried out on the basis of this database to determine the dynamics of diffusion at a given temperature, and thus acquire a complete view of the mechanism of plasticity by diffusion and the conditions (dimensions, temperatures) under which it is favored, as well as the transition to a mechanism of plastic deformation by dislocation nucleation. As the project progresses, it will be possible to study another system (nanowire) or another material (BCC, for example).

Laurent Pizzagalli, Director of Research at CNRS, will formally supervise the thesis. The candidate will also be able to interact closely with a number of local researchers and lecturers, specialists in numerical methods and involved in related research topics. He/she will thus benefit from an ideal scientific environment in which to carry out this thesis. Finally this research topic is the subject of a collaboration with Prof. Felipe Valencia's group at the University of Maule in Talca (Chile). In this context, a stay within this group is conceivable.

[1] Sun et al, Nature Materials **13**, 1007 (2014)
[2] L. Pizzagalli et al, Scripta Materialia 241, 115863 (2024)

Candidate profile

This thesis is based exclusively on numerical simulations, and will be carried out in front of a computer in a Linux environment. To achieve the objectives, you will need to use a variety of numerical tools, and manipulate a large amount of data. This will require the production of small Python codes. You will need to be very comfortable with these tools, and not be allergic to programming in general. Scientific curiosity, analytical skills, synthesis and communication skills are also desirable.

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