Master 2: *Complex Systems*

INTERNSHIP PROPOSAL

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Thesis possibility after internship: YES
Funding: NO

Wise and Efficient Sampling of Plasticity using Atomistic Simulations

The modeling of the plasticity of solids from the atomic scale is still hampered by the accessible time scales - far inferior to those of experiments - and the extreme complexity of the deformation processes [1]. During this internship, it is proposed to solve these two fundamental problems by implementing an original approach based on an automatic saddle point search method informed from the elementary mechanisms of plasticity (i.e. based on a systematic search of the reaction paths according to the mechanisms of plasticity at the atomic scale). Two systems will be studied: 1) nucleation of the dislocations in crystals [2]; 2) plastic rearrangements in glasses [3]. By treating the problems inherent in simulations in radically different solids, crystalline and amorphous, this methodology should allow a scientific breakthrough in the field of modeling the mechanical properties of realistic materials, predominantly and intrinsically complex.

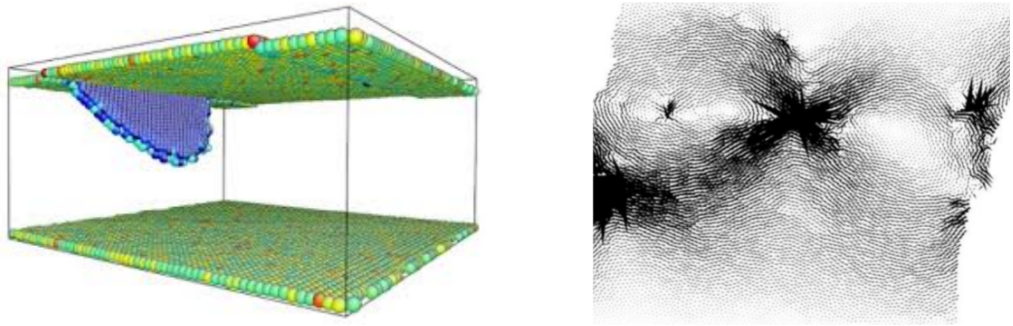

Figure 1: Elementary plastic events. (Left) Nucleation at the surface of a dislocation [2]. (Right) Plastic rearrangement in a glass [3].

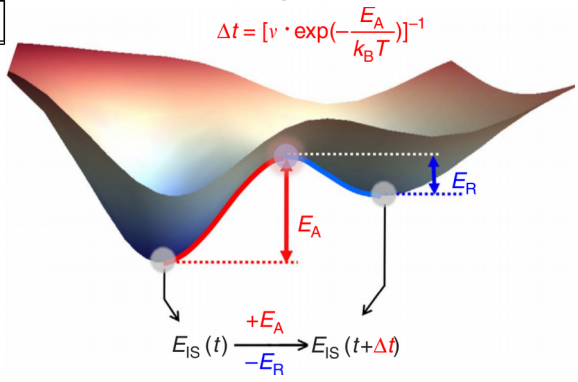

Figure 2: Schematic illustration of elementary hopping in potential energy landscape.

[1] S. Patinet, D. Vandembroucq and M.L. Falk, Phys. Rev. Lett. 117, 045501 (2016)
[2] P. Hirel, J. Godet, S. Brochard, L. Pizzagalli, and P. Beauchamp, PRB **78**, 64109 (2008)
[3] A. Tanguy, F. Leonforte, and J. L. Barrat, Eur. Phys. J. E, **20**, 355 (2006)