

Microscopic understanding of cryogenic rejuvenation

Amorphous materials evolve out of equilibrium in a complex potential energy landscape, and generally undergo a constant evolution in time, called “ageing” that affects their mechanical or thermal properties. The opposite mechanism of “rejuvenation” that brings them to higher energy portions of the energy landscape, can be achieved by mechanical means or by “annealing”, i.e. bringing them to higher temperature for a short period.

In a recent experimental work, Ketov and coworkers¹ reported the surprising observation that rejuvenation can also be obtained by cooling the material in a cyclic manner. This is counterintuitive, as cooling normally only leads to a lowering of the potential energy, i.e. ageing. One possible interpretation of this effect is that amorphous systems have a spatially heterogeneous thermal expansion. As a result, the change in temperature leads to internal mechanical stresses that have the same effect as a macroscopic mechanical treatment.

The aim of the proposed internship is to use numerical simulations of an atomic scale model of a metallic glass to test and validate this hypothesis. The work will involve carrying out simulations according to a protocol that mimicks the experimental one, and to analyse the transformations undergone by the material using microscopic statistical tools.

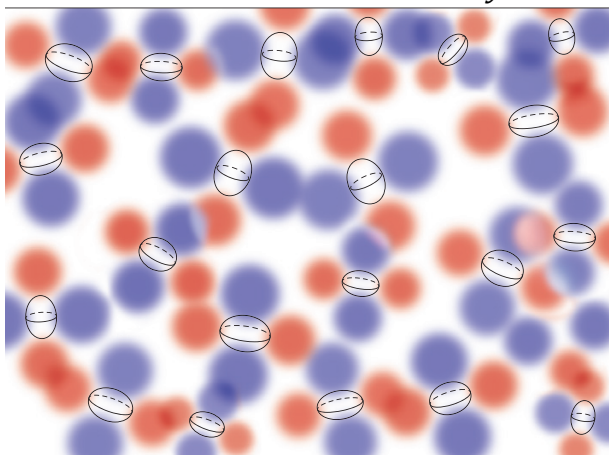
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The proposed internship could take place between March and July and may involve spending a few weeks in Vancouver in the May-June period.

Profile: basic knowledge and interest in simulation tools for condensed matter (Molecular Dynamics, Monte Carlo) ; knowledge of statistical physics, interest in applications to materials science and in disordered systems.



Schematic illustration of the rejuvenation process: blue zones have smaller thermal expansion than red zones, and shrink less upon cooling. As a result, the black ellipses are strongly stressed and undergo mechanical rejuvenation (after T. Hufnagel, Nature Materials, September 2015)

¹ Ketov et al, [Rejuvenation of metallic glasses by nonaffine thermal strains](#), Nature 524, 200(2015)