Tata Institute of Fundamental Research

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Webinar

A statistical mechanical framework for the yielding of ideal crystalline solids

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Crystals, even under infinitesimal shear, eventually yield. This is a consequence of an exact result (by D. Ruelle & M. E. Fisher *et. al.*) that states that the free energy of any material, made up of entities interacting with short ranged forces, cannot depend on the shape of the boundary that becomes irrelevant in the Thermodynamic Limit. Hence the rigid state of a crystal can *at best be metastable* in that limit, implying that a crystalline solid is guaranteed to yield at infinitesimal stresses when deformed at vanishing rates. In this talk, first, I will describe a novel way of classifying atomic displacements, namely, the non-affine projection operator formalism. Within the currently accepted paradigm the atomic displacements are decomposed into smooth (i.e. phonon modes) and singular (i.e. topological defects) components, whereas in our formalism, they are projected onto two mutually orthogonal subspaces. It has been shown that the non-affine subspace acts as a precursor to topological lattice-defects, such as 5-7 defect pairs or stacking faults. Using this formalism, I will show that the yielding phenomena is a dynamic consequence of a hidden first order phase transition, considering an ideal triangular lattice in 2d as the model solid. The free energy of such solids, computed using the Successive Umbrella Sampling (SUS) technique, shows that *the rigid phase of the crystalline solid is metastable* at any finite temperature, under infinitesimal deformation. From this equilibrium picture, the dynamical yield points can be *predicted* as a function of the strain rate using a Classical Nucleation Theory (CNT)-like calculation, and they agree with the rate-dependent yield points that we obtained via Molecular Dynamics (MD) simulations. Then I will show that a closed-form solution to the dynamical yield points can be obtained and numerically solved. The rate-dependent yield points that we take from already published experimental data for tensile loading tests on ultrapure single crystals spanning over 14 orders of magnitudes in strain-rates! Next, I'll describe the 3d counterpart of the problem using an initially defect-free FCC crystal as the model for the solid and I will show that the essential results obtained for the 2d case, remain unchanged. In the quasistatic limit, we find a novel kind of phase transition, namely, the Slip Plane Condensation (SPC) transition that vanishes in the thermodynamic limit. At this point it is worthy to shed some light on the rich geometries of the planar defects formed in the deformed FCC solid that mediates plasticity. Lastly, I will discuss an extension of the CNT for finite strain rates for the 3d case.

Tuesday, Aug 29th 2023

11:30 AM