The crystal road to glass: Non-affine droplet fluctuations in crystalline solids

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Abstract:

A crystalline solid exhibits thermally induced localised non-affine droplets in the absence of an external stress. Upon an imposed shear, the size of these droplets grow until they percolate at a critical strain well below the value at which the solid begins to yield. This critical point does not manifest in bulk thermodynamic or mechanical properties, but is hidden and reveals itself in the onset of inhomogeneities in elastic moduli, disappearance of a metastable liquid-glass spinodal and sudden enhancement in defect pair nucleation with associated structural and dynamical consequences. Introducing a field which couples to non-affine displacements in crystals, enhances non-affine fluctuations and stabilizes the, ordinarily metastable, glassy minima causing a thermodynamic, crystal to glass transition. Many of our results such as single point and two point spatial and temporal correlation functions of non-affine fluctuations and the phase boundary for the crystal to glass transition may be obtained semi-analytically.