

Colloquium

Yielding in crystals towards the quasistatic limit: A slip-plane condensation transition

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When a crystalline solid is slowly deformed with a constant deformation rate, plastic flow initiates only at a limiting deformation called the yield point. In this talk, the yielding of a Lennard-Jones fcc crystal with periodic boundary conditions is studied using particle-based simulation techniques. We show that in the quasi-static limit the yielding can be described as a slip-plane condensation transition, a novel type of first-order phase transition that occurs in the limit of very large but finite linear dimension of the system. This transition shares similarities with the droplet condensation transition^[1, 2] that is observed in the context of first-order phase transitions. It is associated with a jump of an intensive thermodynamic variable and strongly depends on the boundary conditions and the deformation protocol. For finite deformation rates, we present a theory for the deformation rate dependence of the yield strain which is in excellent agreement with the simulation data.

References:

[1] K. Binder, M. Kalos, J. Stat. Phys., 22, 363-396 (1980)

[2] K. Binder, Physica A: Statistical Mechanics and its Applications, 319, 99-114 (2003)

Friday, Feb 23rd 2024

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Auditorium, TIFR-H