Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Students' Annual Seminar

Non-affine fluctuations and the stability of crystalline solids

Pankaj Popli

Long wavelength displacement fluctuations are known to destabilize crystals in two dimensions in the thermodynamic limit. Crystalline solids, in any dimension may also be destabilised by localised, short wavelength, non-affine displacements. These displacements act as precursors for the nucleations of lattice defects [1]. We show how the statistics of these fluctuations may be obtained for a general crystalline lattice in any dimension. We present explicit calculations for the 1d chain, 2d triangular, square, honeycomb and kagome, as well as the 3d simple cubic, bcc and fcc lattices. In each case we show that the non-affine fluctuation mode with the largest eigenvalue (smallest frequency) is associated with lattice defects. In close packed lattices, this mode is separated from other non-affine modes by a large gap in the excitation spectrum. We show how this gap varies from crystal to crystal and also with the degree of coarse-graining. Finally we discuss how such non-affine fluctuations may be suppressed to obtain the stable crystalline solid in the presence of any inter-particle interaction [2, 3, 4].

References:

[1] S. Ganguly, S. Sengupta, P. Sollich, Soft Matter, 11, 4517 (2015).
[2] P. Nath, S. Ganguly, J. Horbach, P. Sollich, S. Karmakar, and S. Sengupta, Proc. Natl. Acad. Sci. USA 115, E4322 (2018).
[3] S. Ganguly, D. Das, J. Horbach, P. Sollich, S. Karmakar, and S. Sengupta, J. Chem. Phys. 149, 184503 (2018). `
[4] P. Popli, S. Ganguly, S. Sengupta, Soft Matter, 14, 104-111 (2018)

Friday, Apr 12th 2019

10:30 AM (Tea/Coffee at 9:30 AM)

Seminar Hall, TIFR-H