Inferring elastic properties of an fcc crystal from displacement correlations: sub-space projection and statistical artifacts

ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We compute the effective dispersion and density of states (DOS) of two-dimensional sub-regions of three-dimensional face centered cubic (FCC) crystals with both a direct projection-inversion technique and a Monte Carlo simulation based on a common Hamiltonian. We study sub-regions of both (111) and (100) planes. For any direction of wavevector, we show an anomalous $\omega^2 \sim q$ scaling regime at low $q$ where $\omega^2$ is the energy associated with a mode of wavenumber $q$. This scaling should give rise to an anomalous DOS, $D_\omega$, at low $\omega$: $D_\omega \sim \omega^3$ rather than the conventional Debye result: $D_\omega \sim \omega^2$. The DOS for the (100) sub-region looks to be consistent with $D_\omega \sim \omega^3$, while the (111) shows something closer to the Debye result at the smallest frequencies. Our Monte Carlo simulation shows that finite sampling artifacts act as an effective disorder and bias the $D_\omega$ in the same way as the finite size artifacts, giving a behavior closer to $D_\omega \sim \omega^2$ than $D_\omega \sim \omega^3$. These results should have an important impact on interpretation of recent studies of colloidal solids where two-point displacement correlations can be obtained in real-space via microscopy.