Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

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 ω^2 is the energy associated with a mode of wavenumber q. This scaling should give rise to an anomalous DOS, D_ω, at low ω: $D_\omega \sim \omega^3$ 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_ω 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.

Asad Hasan
Carnegie Mellon University

Date submitted: 09 Nov 2012

Electronic form version 1.4