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Dynamic and static disorder in supported Pt nanoparticles: when static is not static[1] FD VILA, JJ REHR, U. of Washington, AI FRENKEL, Stony Brook U. — Supported Pt nanoparticles (NPs) exhibit anomalous properties such as negative thermal expansion (NTE) and excessive disorder. Previous finite temperature DFT/MD simulations explain these properties,[2] and show that they arise from bonding heterogeneity both near and far from the support. Pt NPs also exhibit large, so-called "static" or low T disorder, that decreases with increasing size. For small (0.9 nm) NPs, there is significant mean-square bond disorder σ^2, and a fit to an Einstein model results in an anomalously high Einstein temperature (T_E =298±25 K *vs* 179 K in bulk Pt), comparable to Pt-Pt bond strengths in the isolated Pt dimer, as well as an anomalous Gruneisen parameter. To resolve these puzzles, we decompose the σ^2 obtained from DFT/MD runs into "static", dynamic, and vibrational components. We find that the anomalous behavior stems from a decrease in the so-called "static" part with increasing temperature, while the vibrational σ^2 behaves normally with $T_E \approx 179$ K. Finally, we discuss the origin of the pseudo-static σ^2 and Gruneisen parameter, and their temperature dependence, in terms of zero-frequency behavior.

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[2]F.D. Vila *et al.*, Phys. Rev. B **78**, 121404(R) (2008).

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