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Parallel calculations of vibrational properties in complex materials: negative thermal expansion and elastic inhomogeneity.[1] F.D. VILA, J.J. REHR, U. of Washington — Effects of thermal vibrations are essential to obtain a more complete understanding of the properties of complex materials. For example, they are important in the analysis and simulation of x-ray absorption spectra (XAS). In previous work[2] we introduced an *ab initio* approach for a variety of vibrational effects, such as crystallographic and XAS Debye-Waller factors, Debye and Einstein temperatures, and thermal expansion coefficients. This approach uses theoretical dynamical matrices from which the locally-projected vibrational densities of states are obtained using a Lanczos recursion algorithm. In this talk I present recent improvements to our implementation, which permit simulations of more complex materials with up to two orders of magnitude larger simulation cells. The method takes advantage of parallelization in calculations of the dynamical matrix with VASP. To illustrate these capabilities we discuss two problems of considerable interest: negative thermal expansion in ZrW_2O_8; and local inhomogeneities in the elastic properties of supported metal nanoparticles. Both cases highlight the importance of a local treatment of vibrational properties.

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[2]F. D. Vila *et al.* Phys. Rev. B **76**, 014301 (2007).

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