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Mean square atomic displacements of $LaFe_4Sb_{12}$ JOSEPH FELDMAN, Naval Research Laboratory, DAVID SINGH, Oak Ridge National Laboratory — Calculations in the harmonic approximation of the mean square atomic displacements (MSDs) for the filled skutterudite, $LaFe_4Sb_{12}$, are discussed, where the first-principles based force constant model that we recently proposed for this material is employed.[1] The various values of MSDs at high temperatures are as expected, following the differences in coordination and short range force constants. The results are primarily compared with temperature dependent neutron diffraction measurements[2] of MSDs in $La_{.75}Fe_3CoSb_{12}$. The differences between theory and experiment are interpreted in terms of static disorder contributions to the MSDs. In the case of the isotropic MSDs, the resulting static disorder contributions are comparable to the corresponding *minimum* values previously obtained[2] from a data analysis, and both the Sb and Fe values are small compared to the La value of $0.0045 Å^2$. Nevertheless the anisotropy in the Sb static disorder is large on the basis of our analysis, and in the direction of the neighboring La site the Sb disorder parameter is comparable to the above value for La. Finally, the effect of La interactions on the Sb- and Fe-MSDs is discussed within the context of our model, as is an Einstein model, fitted to the calculated La MSD.

1. J.L. Feldman et al., Phys. Rev. B **68**, 094301 (2003).
2. B.C. Chakoumakos et al., Acta Cryst. B **55**,341 (1999).

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