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The Debye-Waller factor and its application to anharmonic vibrations DOUGLAS SAFARIK, ANNA LLOBET, JASON LASHLEY, Los Alamos National Laboratory — The Debye-Waller factor relates the intensities of the Bragg peaks to the mean square displacements of the atoms. In the structural refinement of diffraction data it is standard practice to use the harmonic expression for Debye-Waller factor. For most materials and conditions the phonons are only mildly anharmonic, thus the harmonic assumption is a good one. For some materials and conditions, however, the phonons can be strongly anharmonic, and thus the harmonic assumption is physically unrealistic. As examples we cite the rattling atoms in clathrates and skutterudites, and atoms participating in displacive phase transitions. In the present study we investigate the error associated with using the harmonic Debye–Waller factor to analyze anharmonic vibrations. We find that even for strongly anharmonic potentials, such as a double well, the mean square displacements deduced using the harmonic approximation are at most 15% larger than those deduced using a full anharmonic analysis. Furthermore, the quasi-harmonic and anharmonic values have nearly the same temperature dependences. We conclude that the error introduced by using the harmonic approximation is comparable to or smaller than the usual errors associated with measurement and refinement of diffraction patterns.

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