Holt and Chiang Reply: We would like to thank the authors of the preceding Comment [1], Chou and Choi, for their analysis and insight concerning our Letter [2]. Despite the seemingly straightforward classic analysis of harmonic lattice, there exist disparate definitions and conventions which have led to confusion, and even errors and inaccuracies, in the literature, Equation (1) in our Letter, central to the discussion, is indeed not entirely correct. As discussed in [1], the sum over the two atoms in a unit cell is not shown, and a phase factor seems to be missing. Our discussion in [2] is also hampered by citing erroneous results in the literature. Despite these problems, we would stress that our numerical results and conclusions remain correct. These issues will be clarified below. We will also address the interesting suggestion in [1] of extending our work in a way that will yield the phonon dispersion curves directly without resorting to a fit in terms of a dynamical matrix

The definition of the dynamical matrix presented in [1] is consistent with that of Smith [3], who formulated it in terms of pair force constants up to the second neighbors. This was later extended by Herman [4] to include more distant neighbors for an improved fit to neutron scattering data. However, Patel *et al.* [5] suggested that there was an error in Refs. [3,4]. They asserted that a correction improved the fit, and pair force constants beyond the second neighbors were unnecessary. The dynamical matrix used in our paper was an extension of that in [5] to include up to the sixth neighbors.

This claim of error is actually unfounded. However, the dynamical matrix in [5] is not necessarily wrong either; it simply corresponds to a different (but unspecified) definition:

$$D_{nn'}^{\alpha\beta}(\mathbf{k}) = \frac{1}{\sqrt{\mu_{\mathrm{n}}\mu_{\mathrm{n}'}}} \sum_{\mathbf{R}} D_{nn'}^{\alpha\beta}(\mathbf{R}) \times \exp[-i\mathbf{k}\cdot(\mathbf{R} + \tau_n - \tau_{n'})].$$

The notations used on the right-hand side of this equation are the same as in [1]. Here, the atomic position vectors within the unit cell are included in the lattic Fourier transform, and the dynamical matrix so defined, unlike that in [1], is not periodic in k space. We have verified numerically that the eigenvalues of the dynamical matrix in [5] agree with those in [4], and therefore the "correction" would have no effect on the fit to the neutron data, contrary to the claim made in [5]. The eigenvectors differ, however, by a phase factor arising from the basis. This cancels the phase factor in Eq. (4) in [1], provided the eigenvectors are evaluated at **q**, the full scattering vector, rather than at the reduced vector **k**. Thus, if one takes **q** in Eq. (1) in [2] to be a six-dimensional vector of components $(q_x, q_y, q_z, q_x, q_y, q_z)$ and calculate the inner product with the six-dimensional phonon eigenvector as indicated there, the correct result is obtained. This was the way that we carried out the numerical analysis in [2]. Adding a phase factor in our calculation results in a pattern with features that are qualitatively inconsistent with the experimental results, as would be the case when using an inconsistent set of definitions.

The goal of our project was to develop a simple method for determining phonon dispersions. Chou and Choi have made an excellent suggestion that one could employ different scattering vectors and polarization configurations to probe the same point in k space. The resulting scattering intensities will be proportional to linear combinations of the thermal population factors of the six phonon modes, or a subset of them. These relations can be solved directly to yield the phonon frequencies at the specified point in k space without resorting to a fit of the intensity pattern over a surface in k space. A major advantage of this new approach is mathematical simplicity, and solving a model dynamical matrix equation becomes unnecessary. This is especially useful for complicated systems where an analytic dynamical matrix with sufficient accuracy could be difficult to construct and, in any case, might contain a large number of parameters. We intend to carry out an experiment to test the feasibility of this method.

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