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Temperature-dependence of the forbidden (222) reflection in silicon

Jean Paul Nery ¹ and Philip B. Allen ²

*Physics and Astronomy Department, Stony Brook University,
Stony Brook, NY 11794-3800, USA*

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Abstract

Crystals with an *fcc* lattice like silicon have Bragg scattering at $\mathbf{K} = 2\pi(\mathbf{h}, \mathbf{k}, \mathbf{l})/\mathbf{a}$ for integers hkl all even or all odd. The two-atom basis of the diamond structure causes destructive interference whenever $h+k+l$ is an odd multiple of 2; for example, the (222) reflection is nominally forbidden. However, there is not total interference because of tetrahedral rather than spherical scattering symmetry. Such asymmetry arises from anharmonic vibrations and from bonding. Therefore, the weakly allowed (222) X-ray reflection in silicon is useful for studying bond charge. Temperature variation of the (222) X-ray intensity, beyond that expected from anharmonicity, has been measured [1] and studied [1,2]. Previous theories have been somewhat ad hoc, not dealing fully with electron-phonon induced valence charge density thermal shifts. Namely, the valence charge was assumed to vibrate rigidly around the mid-point of the ions, and Debye-Waller (DW) factors were used. Our formulation of this shift uses full second-order electron-phonon perturbation theory. Both Fan and DW type terms, known to determine band gap thermal shifts, are included. An acoustic sum rule is also used to avoid the computation of electron-phonon matrix elements involving second derivatives of the potential. We compare with experiment and with previous theories.

[1] J. B. Roberto, B. W. Batterman, and D. T. Keating, *Phys. Rev. B* **9**, 2590 (1974).

[2] J. R. Chelikowsky and M. L. Cohen, *Phys. Rev. Lett.* **33**, 1339 (1974)

¹jeanpaul240@gmail.com

²philip.allen@stonybrook.edu