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Harmonic and anharmonic phonons in MgB₂

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The discovery ¹ of a 39 K critical superconducting temperature in MgB₂ has challenged our understanding of electron-phonon mediated superconductivity. Several mechanisms have been proposed to explain the large critical temperature, including a double gap structure and anharmonic effects. Much attention has been devoted to the study of the E_{2g} phonon mode, an anti-phase vibration of the two boron atoms parallel to the hexagonal plane. In Raman spectra ² an E_{2g} symmetry feature, commonly attributed to the E_{2g} phonon mode, is strongly damped, an effect which has been ascribed to large electron-phonon coupling and large anharmonic effects of the E_{2g} mode. The interpretation of the magnitude of each effect is, however, very controversial, mostly because accurate phonon dispersion measurements by neutron spectroscopy are not yet available due to the small size of MgB₂ single crystals.

In this talk we show how the magnitude of anharmonic effects can be determined using a joined experimental and theoretical approach. We measure, for the first time, the phonon dispersion and lifetime in MgB₂ single crystals with inelastic X-ray scattering ³. This experimental technique allows accurate determination of phonon spectra even in the case of small single crystals. By using first principles calculations we obtain the harmonic phonon dispersion in MgB₂ (in agreement with previous calculations ⁴). We evaluate the magnitude of anharmonic effects by calculating the anharmonic contributions to the phonon self-energy. We consider all the lowest order terms from three- and four-phonon vertices. The scattering between different phonon modes at different k-points in the Brillouin zone are included. We use density functional theory and the (2n+1) theorem to evaluate the three- and four-phonon vertices. The inclusion of these terms is found to be crucial in determining the anharmonic contribution to the phonon self-energy. From the real and imaginary part of the phonon self energy we extract anharmonic phonon frequency shifts and linewidths (the inverses of the lifetime) at the special k- points Γ , A, M. We find the anharmonic linewidth of the E_{2g} mode to be negligible compared to that due to electron-phonon coupling. Thus the measurement of the phonon linewidth of the E_{2g} mode allows the experimental determination of the electron-phonon coupling. For the anharmonic phonon frequency shift of the E_{2g} mode we find a cancellation between the contributions of the three- and four-phonon vertices ⁵. The total anharmonic shift of the E_{2g} mode at Gamma is +3.5 meV, corresponding to a relative frequency shift of +5.4%. The resulting anharmonic phonon frequencies are in good agreement with the phonon dispersion measured with inelastic X-ray scattering.

¹J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, and J. Akimitsu, Nature (London) **410**, 63 (2001).

²J. W. Quilty, S. Lee, A. Yamamoto, and S. Tajima, Phys. Rev. Lett. **88**, 087001 (2002)

³A. Shukla, M. Calandra, M. d'Astuto, M. Lazzeri, F. Mauri, C. Bellin, M. Krisch, J. Karpinski, S. M. Kazakov, J. Jun, D. Daghero, and K. Parlinski, Phys. Rev. Lett. **90**, 095506 (2003)

⁴X. Ke, Q. H. Dahn, G. J. Lepp, and G. K. Anderson, Phys. Rev. B **64**, 020501 (R) (2001)