Kohn Anomaly in MgB_2 and Related Compounds by Inelastic X-ray Scattering

MgB_2 has generated an immense amount of interest since its high T_c, ~ 39 K, was first demonstrated a few years ago [1]. This is the highest known critical temperature for a simple metallic material and rather outside the range for T_c using standard estimates. One of the especially interesting properties of MgB_2 is that the electron-phonon coupling (EPC) that causes this high T_c is predominantly to a *particular* phonon mode (with E_{2g} symmetry at Γ), which makes investigating the behavior of this mode very important. Furthermore, the relevant sections of the Fermi surface ("sigma" sheets) are nearly simple cylinders along the c* axis, thus the effects of the electron-phonon coupling should be clear and easy to see in phonon spectra.

A difficulty with MgB_2, however, is that available single crystals are small, ~ 0.01 mm^3, so that the conventional method of investigating phonon dispersion, inelastic neutron scattering, cannot be applied. However, the high brilliance of SPring-8 means that, in principle, such investigations can be carried out with X-rays, assuming a suitable, highly efficient, spectrometer is available. We used the **BL35XU** spectrometer [2], which provides ~ 3×10^{10} photons/s in a 4 meV bandwidth and a small (~100 micron diameter) spot on the sample. Good quality inelastic X-ray scattering (IXS) spectra could be measured from samples of size ~ $0.5 \times 0.2 \times 0.05 = 0.005$ mm^3 in about 12 h, using a 6 meV resolution setup at 15.8 keV (corresponding to the (888) back reflection in silicon).

The EPC of the E_{2g} mode to the sigma surfaces is expected to cause strong softening and a huge increase in the linewidth of the phonon mode as one reduces the in-plane component of the probed momentum transfer from values larger than the diameter of the sigma Fermi surfaces to smaller values. The softening is an extreme example of a Kohn anomaly, while the broadening corresponds to the reduction in phonon lifetime that occurs as the additional decay channel (excitation of the electronic system) turns on at smaller momentum transfers. The momentum transfer dependence is easily understood qualitatively based on the shape of the sigma Fermi surfaces: since phonon energies are negligible on the

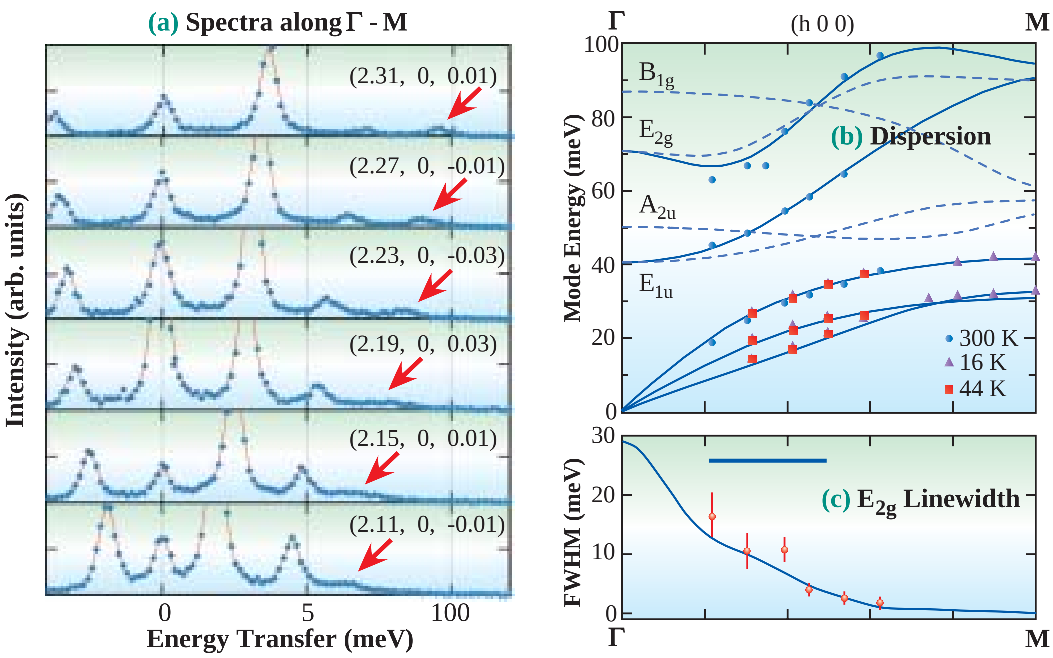

Fig. 1. Phonon dispersion in pure MgB_2 (see [3]).
(1a) Selected IXS spectra (room temperature) with fits (solid lines). The softening and broadening of the E_{2g} mode (indicated by red arrows) are readily apparent. **(1b)** Phonon dispersion determined by fits to the data (points) and the results of *ab initio* calculations (lines - Bohnen *et al.*, Phys. Rev. Lett. **86** (2001) 5771; dashed lines are modes not expected to be observed from phonon polarization considerations). **(1c)** Measured linewidth after correction for resolution, and the theoretical calculation (see text). In general, there is excellent agreement with the theoretical calculation. The solid horizontal bar shows the diameter of the sigma Fermi surfaces projected into the basal plane which is the expected position for the Kohn anomaly.

scale of most electron states, EPC is only possible for phonons with momenta appropriate to move electrons within the neighborhood of a Fermi surface. Given the nearly circular projection of the sigma surfaces into the basal plane, small phonon momenta can move electrons from one location to another across the Fermi surface. However, for larger momenta ($Q > 2\,k_F$), all appropriate states are filled, thus the coupling is reduced. Figure 1 shows the results from a pure MgB_2 sample along the ΓM line [3] of the basal plane – the softening and broadening as one moves inside the sigma surfaces are immediately clear. Furthermore, the agreement with theoretical calculations is excellent, both in dispersion and linewidth, even for this very extreme case of strong coupling of single mode. This provides crucial confirmation that MgB_2 is an extreme case of a conventional BCS / Eliashberg-type superconductor.

Having demonstrated the effects of the EPC on the E_{2g} mode and their good agreement with theoretical results, we tried to modify the sample a bit; the recent growth of single crystalline carbon-doped $Mg(B_{1-x}C_x)_2$ [4] provides an excellent opportunity. In particular, the sigma sheets of the Fermi surfaces are hole surfaces, so that electron doping with C can be expected to close them and remove the electron phonon coupling. Thus, we investigated the behavior of the E_{2g} mode in samples with 2%, 5% and 12.5% carbon doping, corresponding to transition temperatures of 35.5, 30 and 2.5 K, respectively. The softening remains clear in the 2% and 5% samples; however, as evident in Fig. 2, in the 12.5% sample, the softening goes away, and the E_{2g} mode "pops up", showing the removal of the EPC from these surfaces. This is in good agreement both with expectations regarding the changes in T_c and with one calculation suggesting that about 9% carbon doping should be sufficient to fill the sigma bands.

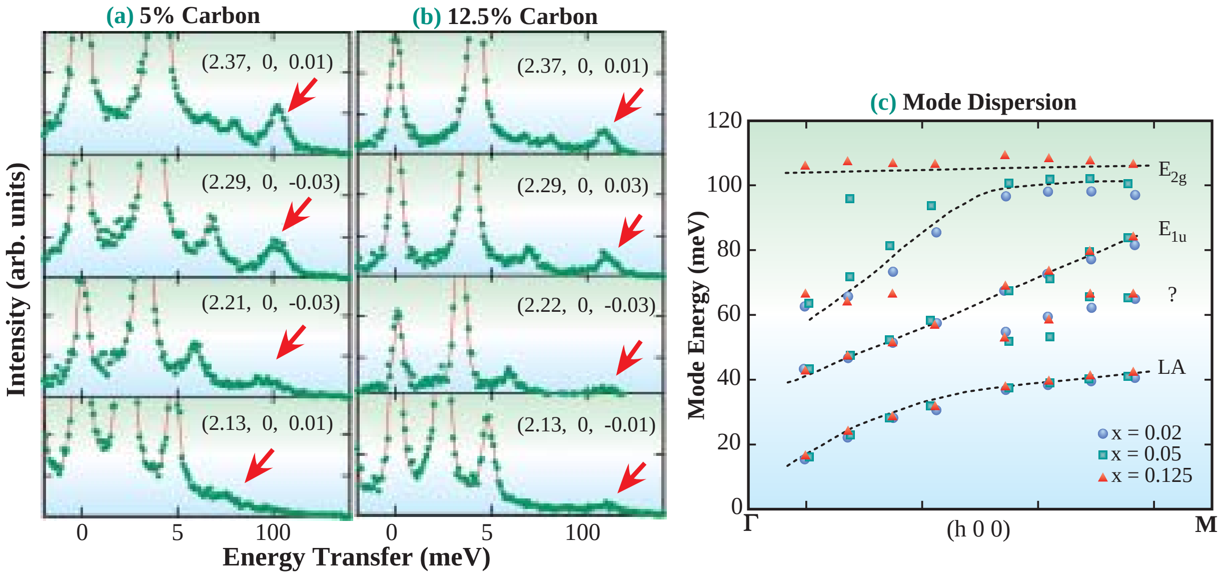

Fig. 2. Phonon dispersion in carbon-doped material, $Mg(B_{1-x}C_x)_2$ [5]. Selected IXS spectra (room temperature) with fits (solid lines) from **(a)** x = 0.05 sample and **(b)** x = 0.125 sample. **(c)** shows the phonon dispersion determined from the fits and a guide to the eye (dashed lines). The E_{2g} mode "pops up" when the carbon content is increased to 12.5%, as expected from filling the sigma surfaces. The presence of the extra mode evident at higher momentum transfers and other details are being analyzed

Alfred Q.R. Baron[a] and Hiroshi Uchiyama[b]

(a) SPring-8 / JASRI
(b) Superconductivity Research Laboratory, ISTEC

E-mail: Baron@spring8.or.jp

References

[1] J. Nagamatsu *et al.*: Nature **410** (2001) 63.
[2] A.Q.R. Baron *et al.*: J. Phys. & Chem. Solids **61** (2000) 461.
[3] A.Q.R. Baron, H. Uchiyama, Y. Tanaka, S. Tsutsui, D. Ishikawa, S. Lee, R. Heid, K.-P. Bohnen, S. Tajima and T. Ishikawa: Phys. Rev. Lett. **92** (2004) 197004.
[4] S. Lee *et al.*: Physica C **397** (2003) 7.
[5] A.Q.R. Baron, H. Uchiyama, S. Tsutsui, S. Lee and S. Tajima: in preparation.