ESRF

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Electron-phonon coupling and anharmonicity in MgB2: temperature effects and low q lifetime	HS-2598

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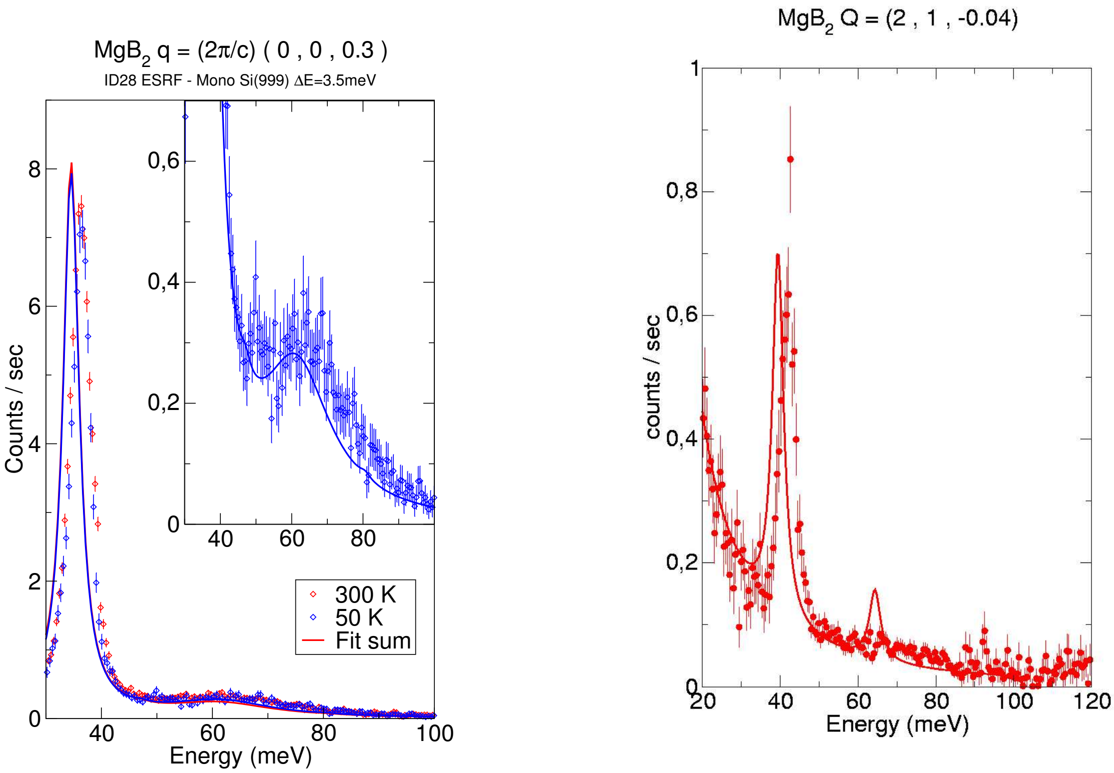
Report:

The discovery of high critical temperature (T_c = 39K) in MgB_2 has challenged our understanding of electron-phonon coupling mediated superconductivity. Much attention has been devoted to the study of the E_{2g} phonon mode. This mode has the largest coupling with electrons according to our previous inelastic X-ray scattering measurements at ESRF on ID28 (1) and plays a crucial role in the determination of the superconducting properties of MgB_2. The E_{2g} mode has also been associated with a supposedly large anharmonicity, which, according to some authors, is related to the special role played by this mode in the occurence of the high T_c in MgB_2 (see *e.g.* 2). However, quantitative determination of the anharmonic effects has led so far to controversial results (see the detailed discussion by Lazzeri *et al.* in the introduction of Ref. 3). In particular, some theoretical calculations indicate the anharmonic frequency shift of the E_{2g} mode at Γ to be large, with varying estimates that range from +15%, up to +20/25% of the theoretical harmonic frequency ($\sim$ 65 meV). A comparably large shift is expected to affect this mode all along the Γ-A direction. Raman measurements (see Ref. 4 and references therein) seem to confirm the prediction of a large anharmonicity at Γ. Moreover, Raman spectra display a drastic dependence on the temperature (see Fig. 2). The width of the 77 meV peak is $\sim$ 20 meV at T= 40K and reaches almost 40 meV at room temperature (4). This behaviour has been tentatively attributed to anharmonicity (Ref. 4 and references therein), but, according to the calculations of Ref. 1, the E_{2g}-Γ anharmonic broadening at room temperature is negligible, just 1.2 meV. Moreover, even the prediction of a strong anharmonic frequency shift is in stark contrast with the inelastic X-ray measurements

of the MgB_2 phonon dispersion of Ref. 1, which E_{2g} phonon frequencies measurements are in agreement (within 5%) with the calculated harmonic phonon frequencies (1) at several points along the Γ-A direction.
Therefore we decided to probe the E_{2g} with high energy and Q resolution, in function of temperature and close to Γ with ixs, in the experiment related here.



Left panel *IXS data (diamond) and ab-initio simulation (lines) at 0.6×Γ-A for T=300 K (red point and line) and T=50 K (blue point and line). Inset: data and calculation at 50 K.*
Right panel *Room temperature IXS data at 0.08×Γ-A, the line is an ab-initio simulation convoluted with the resolution, with no* ***electron-phonon*** *coupling broadening effect on the E_{2g} mode.*

Conclusions

The data show evidence that the temperature dependence of the E_{2g} lifetime along Γ-A is well accounted by our model at least at the A point (data not shown here) and 0.6×Γ-A. However, we where not able to clearly show the effect close to the Γ, which seems to point out to a broadening still large as close to Γ as 0.08×Γ-A. Data are under analysis in order to take in to account temperature background effect coming from static diffuse scattering close to the zone centre.

1. A. Shukla *et al., Phys. Rev. Lett.* **90**, 095506 (2003).
2. T. Yildirim *et al., Phys. Rev. Lett.* **87**, 037001 (2001)
3. M. Lazzeri *et al., Phys. Rev. B* **68**, 220509 (2003).
4. J.W. Quilty *et al.*, Phys. Rev. Lett. **88**, 087001 (2002).