ESRF	**Experiment title:** Non-adiabatic effects in the phonon dispersion of MgB_2	**Experiment number**: HS-4802
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Report:

Our aim in this experiment is to measure a direct effect of *non-adiabatic electron-phonon* coupling on the phonon dispersion of MgB_2.

These effects have been invoked to explain an apparent contradiction between the energy shift and broadening of the phonon signal found using conventional Raman scattering and the ones using Inelastic X-ray Scattering (IXS). This is important for the theory of superconductivity of MgB_2, as an alternative interpretation of the Raman shift and broadening, in term of anharmonicity, could explain the anomalous isotopic effect of MgB_2, but not the IXS shift and broadening. Moreover, there are very few experimental confirmation of non-adiabatic effects in solids, even if they can be relevant in the interpretation of vibrational data and the electron-phonon coupling of various layered metals as intercalated graphite and graphene and, in general, for metals characterized by a small Fermi velocity in a particular direction.

Our experiment on id28 shows, that the dispersion bend up approaching the zone centre, as it illustrated in Fig. 1. Indeed, a rough extrapolation to the Gamma point indicates that there is a continuous increase of the phonon energy up to the value found by Raman experiment. This is a great achievement, as in a previous

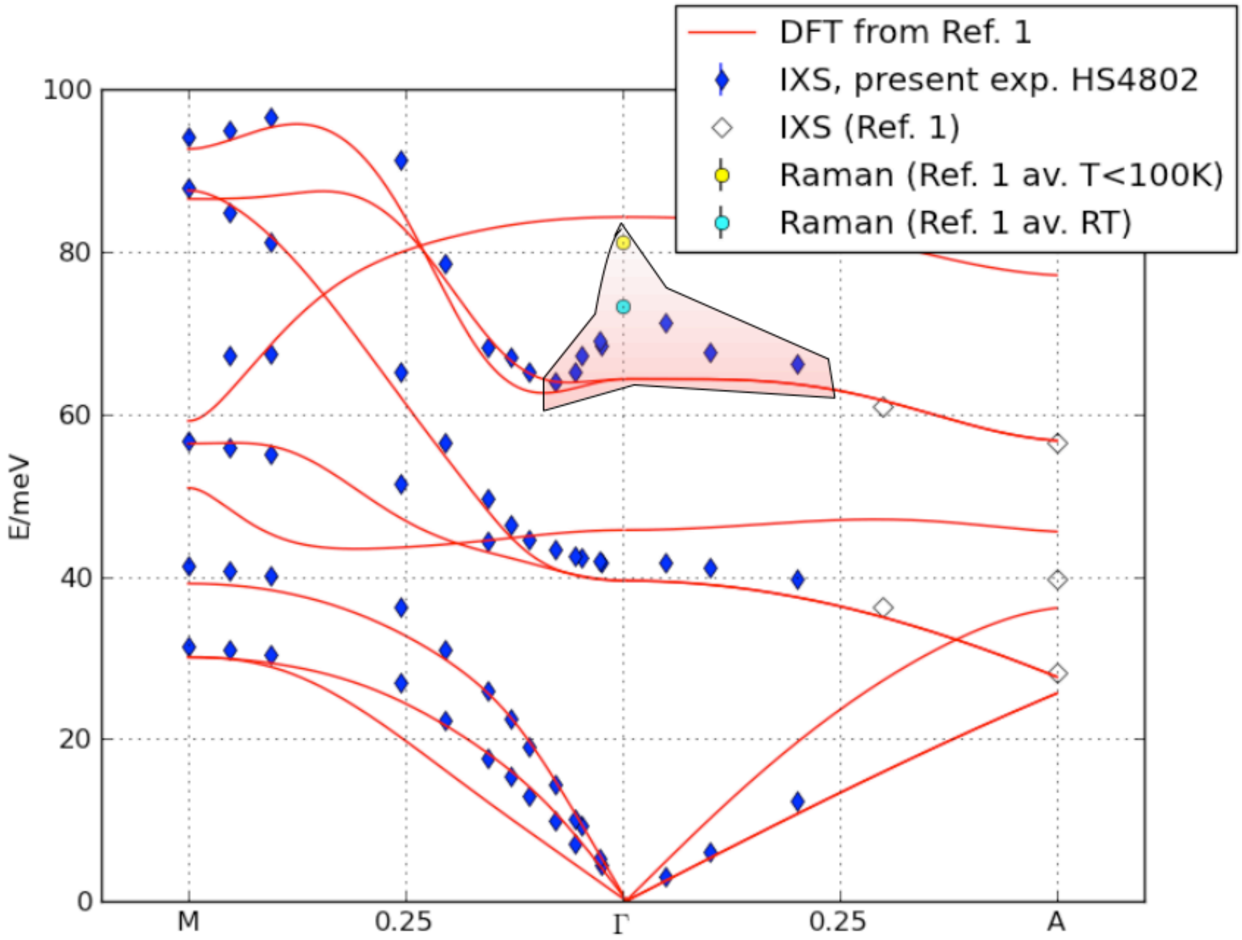

Fig. 1: Phonon dispersion in MgB2 along GA and GM, measured by IXS (diamonds), compared to DFT simulation (lines, from Ref. 1) and Raman, at RT and below 100 K (circles, from Ref. 1). Error-bars on energy are not visible when smaller than the marker size. The anomalous E2g dispersion at Γ is highlighted by gradient filled area.

experiment (1), on the same crystal, it was impossible to get any signal, with the tighter resolution condition required to approach the zone centre and describe the details of

the dispersion on a scale of few hundredths of the Brillouin zone. This achievement become possible today thanks to the constant improvements of the beam-line, allowing a gain in brilliance large enough to compensate the loss due the smaller angular acceptance of the scattered photons. The Flux and brilliance gain allowed affording better Q-resolution, and therefore measure more close to the Brillouin Zone Center with small steps in the reciprocal space, necessary for this very steep dispersion.

We are currently comparing the data to older IXS and Raman data on doped $(Al,Mg)B_2$ data from the Karlsruhe group, possibly in order to understand how this effect evolve from the adiabatic case in AlB_2, in view of the preparation of an article.

References

1) M. d'Astuto, M. Calandra, S. Reich, *et al. Phys. Rev. B* **75**, 174508 (2007)