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# Phonon softening in $HgBa_2CuO_{4+\delta}$ and $MgB_2$

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**Abstract**

Phonon dispersion of two superconductors was studied with using inelastic X-ray scattering. In $MgB_2$, which is thought as a Eliashberg type superconductor, the phonon dispersion shows softening of the $E_{2g}$ mode around Γ in the [100] direction, in excellent agreement with ab initio calculations. It supports the idea that this phonon gives main contribution to the superconductivity. In $HgBa_2CuO_{4+\delta}$, on the other hand, which is a good candidate for phonon measurement in the high-$T_c$ cuprates, the dispersion shows anomalous softening of the bond stretching mode at $q \sim 0.3$ in the [100] direction. The softening does not agree with shell model calculations well, suggesting existence of spatial charge fluctuation with periodicity of $q \sim 0.3$.


*Keywords:* A. Superconductors; D. Phonons

## 1. Introduction

Investigation of phonons in superconductors is an interesting issue, with respect to the electron–phonon interaction. In conventional BCS superconductors, the phonon plays a crucial role in the superconductivity. In superconductivity of high-$T_c$ cuprates, on the other hand, the role of electron–phonon coupling has been unclear, probably because the strong electron correlation may affect the phonon behavior.

Phonon dispersion has been mainly studied by inelastic neutron scattering, which requires a large crystal with a size of $\sim 1\ cm^3$. Recent development of synchrotron radiation and the inelastic X-ray scattering (IXS) technique [1] enabled us to measure phonon dispersions even for small samples (much less than $1\ mm^3$). We report here the IXS results for the two superconductors, $MgB_2$ and $HgBa_2CuO_{4+\delta}$ (Hg1201)[2,3].

$MgB_2$ has a simple hexagonal structure which consists of two-dimensional honeycomb boron network sandwiched by Mg-layer, and has a high superconducting transition temperature, $T_c \sim 39$ K. There are two types of bands, B $\sigma$ bands and B $\pi$ bands, crossing the Fermi level. The $\sigma$ bands have mostly cylindrical structure, while the $\pi$ bands three-dimensional character. The superconductivity is well described in phonon-mediated mechanism, resulted from strong coupling between the $\sigma$ bands and the boron vibration mode with $E_{2g}$ symmetry.

$HgBa_2CuO_{4+\delta}$ (Hg1201) is a good candidate for phonon studies in the high-$T_c$ cuprates. The crystal structure is tetragonal, forming a completely square and flat $CuO_2$ plane. Moreover, the absence of the 1/8-anomaly suggests that the static stripes play no role in Hg1201[4]. Hg1201 is also interesting because the structure is similar to LSCO, while $T_c$ ($\sim 98$ K) is similar to YBCO.

## 2. Experiment

Single crystal $MgB_2$ samples were prepared under high-pressure of 4–6 GPa [5]. A typical size is $0.2 \times 0.5 \times 0.05\ mm^3$, and magnetic susceptibility measurements verified that the crystals exhibit superconductivity at $\sim 38$ K with a narrow transition width of 0.3 K. Single crystals Hg1201, on the other hand, were prepared with a solid-state reaction method [4]. The crystal has the size of $0.3 \times 0.3 \times 0.2\ mm^3$, and magnetic susceptibility measurement showed a superconductivity transition at 94 K. Before IXS measurements, crystallinity of each

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sample was examined by X-ray diffraction and there was no trace of detectable impurity phase.

The IXS measurement achieved at BL35XU of SPring-8 [1] with using the Si (888) (=15.816 keV) (both for $MgB_2$ and Hg1201) and Si(11 11 11) (=21.747 keV) (for $MgB_2$) reflections. Due to the short attenuation length of X-ray for Hg1201, Si(888), which provides $\sim 3\times 10^{10}$ photons/s, was selected instead of Si (11 11 11)($\sim 3\times 10^{9}$ photons/s) in the measurement. The overall resolution, which is determined by using a standard poly methyl methacrylate sample, is 1.6–1.8 meV for Si (11 11 11), while 6.0–6.3 meV for Si(888). The beam size at the sample is about $0.1\times 0.1$ mm$^2$ in the FWHM (full width at half maximum).

## 3. Results and discussion

### 3.1. $MgB_2$

Fig. 1 shows the spectra of $MgB_2$ along ΓM (M=($\pi$,0,0)) taken at room temperature. In this configuration, besides elastic peak locating at $E=0$, we can see three peaks in each momentum as Stokes lines (LA (longitudinal acoustic), $E_{1u}$, $E_{2g}$). As a summary of several configurations and temperature conditions, Fig. 2(a) shows the phonon dispersion. For the $E_{2g}$ mode, the $q$-dependence of line-width is also plotted in Fig. 2(b) determined by fitting. The lines in Fig. 2 are the calculation using a mixed-basis pseudopotential method, combining the plane waves and the local functions for the valence states [6]. The dashed line in Fig. 2(a) means the dispersion which is not available (or weak scattering cross section) in the applied configuration.

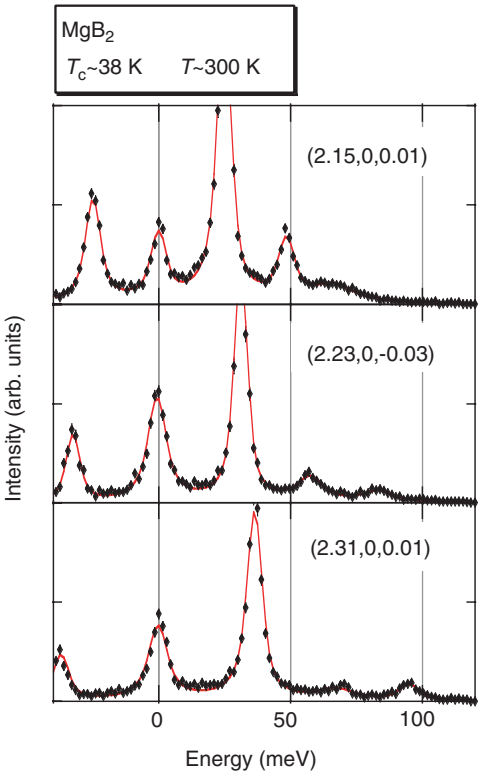


Fig. 1. IXS spectra for $MgB_2$ in the ΓM direction. Room temperature (~300 K) and 6 meV resolution. Solid line is fit to the data.

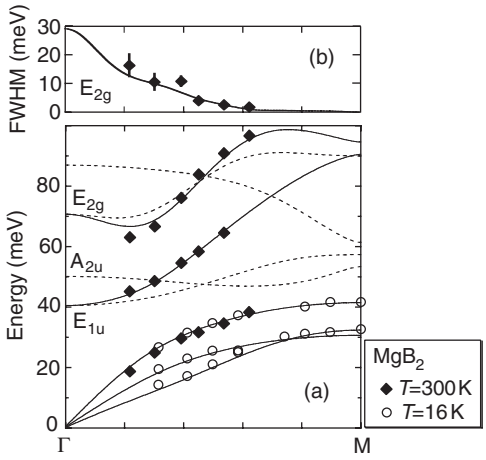


Fig. 2. (a) Phonon dispersion for $MgB_2$. Points show measured values while lines are calculations of Ref. [6]. Dashed lines show branches not investigated in this work due to polarization selection rules or choice-of-scan range. The data at room temperature were taken with the Si(888) reflection, while the data at 16 K with the Si(11 11 11) reflection. (b) Measured and calculated $E_{2g}$ line-width.

In Figs. 1 and 2, we can see the softening and the broadening of the $E_{2g}$ mode (the branch in the highest energy in Fig. 1) when approaching Γ. Such features are well understood as a result of Kohn anomaly of the $E_{2g}$ mode interacting with the $\sigma$-Fermi surfaces, which are mostly cylindrical with $c^*$-axis (radius ~0.14 and 0.21 ΓM). Comparing the experiment to the calculation, we found that the calculation [6] well explains both of the softening (Fig. 2(a)) and the broadening (Fig. 2(b)) [1]. The present result provides a firm evidence for the scenario that the $E_{2g}$-mode strongly couples with the electronic system and thus plays a crucial role in superconductivity pairing.

### 3.2. $HgBa_2CuO_{4+\delta}$

Fig. 3 shows the spectra of Hg1201 along ΓX (X=($\pi$,0,0)) in the longitudinal mode. In this configuration, the $\Delta_1$-symmetry phonon modes, which includes eight branches in Hg1201, should have strong scattering cross section (LA, $2\times A_{1g}$ ($c$-polarized), and $5\times E_u$ ($a$-polarized) at Γ). Compared to the spectra of $MgB_2$, the elastic peak has strong spectral intensity in Hg1201, because Hg1201 contains heavy elements (Hg and Ba). To remove the effects of the elastic peak, the elastic peak obtained from the standard material was subtracted at each momentum, in fitting (insets in Fig. 3). Some of the eight phonon branches are not detected, because of the weak intensity.

In contrast to the calculation of phonon dispersion for $MgB_2$, ab initio calculation for Hg1201 is quite difficult due to presence of a heavy element (Hg) and the large unit cell. In order to simulate the measured spectra, instead of ab initio calculation, we used a simple shell model calculation [3],