Lattice dynamics and magneto-elastic coupling in Kondo-insulator YbB$_{12}$

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Abstract. Lattice dynamics and magneto-elastic coupling effects have been studied in the Kondo insulator YbB$_{12}$ by means of inelastic neutron scattering. The analysis of the phonon density of states, dispersion, and symmetry properties is presented in connection with a possible magneto-elastic coupling. Manifestation of such effects was found for the phonons corresponding to the vibrations of Yb atoms.

1. Introduction

Kondo-insulators form a specific class of the rare-earth compounds which behave as Kondo metals at room temperature and transform to narrow-gap semiconductors with a non-magnetic ground state on decreasing temperature [1]. YbB$_{12}$ is a typical Kondo-insulator and the only example reported so far among Yb-based compounds. It is of particular interest because of its crystal structure formed by a rigid network of boron cuboctahedra B$_{12}$ and loosely-bound Yb ions. Inelastic neutron scattering (INS) experiments on YbB$_{12}$ have revealed that the spin-gap formation on cooling below 80 K [2,3] is also accompanied by the formation of near-gap-edge dispersive magnetic excitations [4]. The conventional approach to the Kondo-insulator problem is based on the consideration of strong f-d hybridization. However one should not exclude the possible interplay between electron and lattice excitations, at least in case of YbB$_{12}$ where collective magnetic excitations (characteristic for the low-temperature Kondo-insulating regime) fall in the same energy range as phonons associated with rare-earth ion vibrations. Since the structure of the magnetic excitation spectrum itself is strongly temperature-dependent such magneto-elastic coupling (MEC) effects can become especially evident when studying the temperature evolution of phonon spectra.

In this paper we present the results of an INS study of the phonon density of states (PhDOS) and dispersion curves in YbB$_{12}$ (partly published in [5,6]), along with possible evidence for MEC effects.

2. Phonon density of states

Previously [2], we have studied phonon spectra of YbB$_{12}$ and its nonmagnetic structure analogue LuB$_{12}$ on powder samples by means of INS. It was found that, owing to the small difference in mass between Yb and Lu and to the closeness in lattice constants, the phonon spectra in these compounds
are quite similar. Therefore, it is possible to apply the isotope contrast method [7] for refining the PhDOS from the experimental INS spectra. Thus, we have obtained the total and partial (for Yb and B) PhDOS in YbB$_{12}$ at $T = 159$ K as shown in Figure 1(d). The vibrational spectra of the RE atoms have considerable localized character with only one pronounced peak at about 15 meV whereas boron vibrations extend over the whole spectral range up to the cutoff energy (~135 meV). From the partial PhDOS we calculated the average force constants $\langle B_\nu \rangle = \frac{M}{\hbar} \int_g (\omega)(h\omega)^2 d\omega$. It is found that the average bonding strength with the crystal lattice for Yb is about 30 times less then for boron atoms.

![Figure 1](image)

**Figure 1.** (a)-(c): Phonon dispersion curves in YbB$_{12}$ (open symbols) and LuB$_{12}$ (closed symbols). Circles: longitudinal branches; diamonds: transverse branches. The results of the model calculation are shown as solid lines [5]. Symmetries of phonons are labeled according to Bouckaert-Smoluchowski-Wigner notations [8].

(d): PhDOS in YbB$_{12}$. Hatched area: boron partial PhDOS, Crossed-hatched pattern: ytterbium partial PhDOS.

### 3. Phonon dispersion curves

Phonon dispersion in the Kondo-insulator YbB$_{12}$ and its structural analogue LuB$_{12}$ was studied at room temperature up to 55 meV [5] (figure 1(a-c)). As expected from the measurements on polycrystalline samples, the phonon energies in YbB$_{12}$ and LuB$_{12}$ do coincide within experimental accuracy. For both compounds, transverse and longitudinal acoustic branches have large flat parts at about 15 meV and are almost degenerate. Optic branches are separated from acoustic ones by a gap of the order of 5 meV. Just near the gap-edge an almost dispersionless optic branch is observed. All these peculiarities are clearly reflected in the structure of the PhDOS (see Figure 1). Phonon dispersion and PhDOS were successfully described in terms of Born–von-Karman force constant model based on the strong hierarchy of interatomic interactions: Yb–Yb $\ll$ Yb–B $\ll$ B–B [5] in agreement with the data obtained from the partial PhDOS analysis. The model describes quantitatively the dispersion of acoustic branches and the energies of optic branches at Brillouin zone centre. It also gives a qualitative
description of the low-energy optic branches over the whole Brillouin zone, as well as the dynamic structure factors for all branches measured. An important point of the model treatment is the symmetry analysis of the measured phonons, which makes it possible to select the branches that might be affected by MEC (see next section).

4. Magneto-elastic coupling effects

The most promising candidates for the observation of MEC effects are acoustic branches associated mainly with Yb vibrations (see figure 1(d)). We therefore searched for evidence of MEC in the evolution of the low-energy phonon peak ($E \approx 15$ meV) going through the transition from the high temperature metallic regime to the low-temperature Kondo-insulating state. We have analyzed INS spectra measured at large $Q$ values (more than $9 \text{ Å}^{-1}$). At such large momentum transfers, magnetic scattering in YbB$_{12}$ is negligible and the experimental spectra can thus be considered as purely phononic in origin.

![Figure 2](image_url) Parameters of the low-energy phonon peak in YbB$_{12}$ spectra as a function of temperature: (a) phonon peak width (circles) and energy (triangles), (b) experimental intensity corrected for Bose factor (stars); dashed line - behavior of the phonon intensity according to normal Debye-Waller factor.

The ytterbium phonon peak energy appears to be temperature-independent, and its width slightly increases upon heating (see figure 2(a)). At the same time, the integrated intensity of the phonon peak shows a remarkable increase at low temperatures (after correcting for the Bose factor). This effect is much stronger than could be expected from the normal behavior due to the Debye-Waller factor (calculated using partial PhDOS and shown in figure 2(b)). Such a behavior could be related to the renormalization of phonon eigenvectors. We can ascribe it to the magneto-elastic coupling especially in view of the fact that the upturn in the intensity temperature dependence takes place at a temperature close to the crossover into the Kondo-insulating regime.

To justify this assumption a detailed single-crystal study of the temperature dependence of specific phonon modes, along with a symmetry analysis for both phonon and magnetic excitation, is needed. If we suppose that magnetic excitations in YbB$_{12}$ are of the same symmetry as the crystal-field excitations (irreducible representation $\Gamma_{25}'$ in Bouckaert-Smoluchowski-Wigner notations [8]) it is possible to select phonons that can interact with magnetic excitations. According to the compatibility...
relations, along high-symmetry directions [001], [110] and [111] representation $\Gamma_25'$ splits into $\Delta_5' \oplus \Delta_5$, $\Sigma_1 \oplus \Sigma_3$, $\Lambda_1 \oplus \Lambda_3$ respectively. For Yb phonons we have the following representations: $\Gamma_{15}$, $\Delta_1 \oplus \Delta_5$, $\Sigma_1 \oplus \Sigma_3$, $\Lambda_1 \oplus \Lambda_3$. Therefore $\Delta_5$, $\Sigma_1$, $\Sigma_3$, $\Lambda_1$, and $\Lambda_3$ phonons can be expected to participate in MEC. Indeed, preliminary measurements on a single crystal revealed an anomalous temperature dependence of phonon intensities for the branches of $\Sigma_3$ and $\Lambda_1$ symmetry, similar to the behavior observed on polycrystalline samples.

5. Conclusion

The study of lattice dynamics in the Kondo insulator YbB$_{12}$ has been presented. We have obtained the total and partial phonon densities of states, and analyzed the dispersion curves at high temperatures (159K and room temperature, respectively). The low-energy lattice dynamics in YbB$_{12}$ is found to be governed mainly by the acoustic vibrations of loosely-bound Yb atoms. Phonon peaks associated with Yb vibrations have an anomalous temperature dependence of their intensity. The effect is ascribed to magneto-elastic coupling between lattice and magnetic excitations. This possibility is supported by the results of the symmetry analysis of the corresponding phonon branches.

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