Superconductivity in MgB₂: Magneto-Raman Measurements

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Abstract. Polarization-resolved Raman scattering measurements of MgB₂ superconductor as function of excitation, temperature and magnetic field have revealed four distinct superconducting features: a clean gap below 35 cm⁻¹ and three superconducting coherence peaks at 50 and 110 cm⁻¹ for the E_{2g} symmetry and at 75 cm⁻¹ for the A_{1g} symmetry. Their temperature and field dependences have been established. Superconductivity induced renormalization of the E_{2g} phonon consistent with electron-phonon coupling $\lambda \approx 0.3$ has been observed.

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The two superconducting (SC) gaps nature of MgB_2 is experimentally established by a number of spectroscopies. The SC gaps have been assigned to distinctive (σ - and π -band) Fermi surface (FS) sheets by means of ARPES [1]. The larger gap, $\Delta_{\sigma} = 5.5 - 6.5 \text{ meV}$, is attributed to σ -bonding states of the boron $p_{x,y}$ orbitals and the smaller gap, $\Delta_{\pi} = 1.5 - 2.2 \,\text{meV}$, to π -states of the boron p_z orbitals. Scanning tunneling microscopy (STM) has provided a reliable fit for the smaller gap, $\Delta_{\pi} = 2.2 \,\text{meV}$ [2]. This value is close to the absorption threshold energy $2\Delta_0 = 31 \text{ cm}^{-1}$ obtained from magnetooptical far-IR studies [3]. The nominal upper critical field H_{c2}^{π} deduced from the coherence length $\xi_{\pi} = 49.6$ nm by vortex imaging is $H_{c2}^{\pi} \approx 0.13$ T [2] that is much smaller than the critical field $H_{c2}^{optical} \approx 5$ T found by magnetooptical measurements [3]. To explain near 40 K SC T_c in MgB₂ a large, in order of unity, electron-phonon coupling constant λ is required [4]. This coupling is expected to manifest itself in strong self-energy effects across the SC phase transition.

Raman scattering from the *ab* surface of MgB₂ single crystals with $T_c \approx 38$ K was performed in back scattering geometry using circularly polarized light. The data in magnetic fields was acquired with a continuous flow cryostat inserted in the horizontal bore of a superconducting magnet. We used the $\lambda_L = 482.5$ and 752.5 nm excitation lines of a Kr⁺ laser and a triple-grating spectrometer for the analysis of the scattered light.

In Fig. 1 we show evolution of the SC coherence peaks for both the E_{2g} and the A_{1g} scattering channels across the SC transition for two cases: varying temperature at zero magnetic field (a, c) and varying the magnetic field at 8 K (b, d). The coherence peaks lose their intensity and move to lower energies by either increasing the temperature or field. In the SC state we observe a clean threshold of Raman intensity, $2\Delta_0 = 35$ cm⁻¹ for all



FIGURE 1. Evolution of low-frequency Raman response as function of temperature at zero field (a,c) and field at 8 K (b,d). The E_{2g} channel, right-left (*RL*) polarization, with λ_L = 482.5 nm excitation is shown in (a,b) and the A_{1g} channel, right-right (*RR*) polarization, with λ_L = 752.5 nm in (c,d).

scattering geometries. This threshold appears along with two SC coherence peaks in the E_{2g} scattering channel, $2\Delta_L^E = 110 \text{ cm}^{-1}$ and $2\Delta_S^E = 50 \text{ cm}^{-1}$, and another peak in A_{1g} channel, $2\Delta^A = 75 \text{ cm}^{-1}$. The energy scales Δ_0 and Δ_L^E are consistent respectively with Δ_{π} and Δ_{σ} from one-electron spectroscopies [1, 2].

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FIGURE 2. Phononic self-energy effect due to SC transition. Evolution of the Raman response in the E_{2g} channel (RL) across the SC transition as function of temperature in zero field (a) and as function of field applied parallel to the *c*-axis at 8 K (b), $\lambda_L = 482.5$ nm. The data (dots) are fitted (solid line) with two phononic oscillators and SC coherence peak on electronic continuum (decompositions for the lowest spectra are shown). The E_{2g} phonon frequency $\omega(T,H)$ and the damping constant $\Gamma(T,H)$ are drawn as functions of temperature (c) and field (d). In (c) zero field cooling (solid symbols) and 7 T cooling (empty symbols) are shown. The low temperature limit of ω_0^{S} and ω_0^N are approximated for corresponding cooling. Solid line is fit in normal state to a model of anharmonic decay, $\Gamma(T) = \Gamma_0 + \Gamma_3 [1 + 2n(\Omega/2)] + \Gamma_4 [1 + 3n(\Omega/3) + 3n^2(\Omega/3)].$ Here $\Omega(T) = hc\omega_h/k_BT$, harmonic frequency $\omega_h = 515 \text{ cm}^{-1}$ [5, 6], *n* is the Bose-Einstein distribution function, the internal temperature independent line width Γ_0 is small, $\Gamma_3 = 190$ and $\Gamma_4 = 20 \text{ cm}^{-1}$ are broadening coefficients due to the cubic and quartic anharmonicity. Since $\Gamma_3+\Gamma_4\gg\Gamma_0$ we conclude that the anharmonic decay is primarily responsible for the large damping constant of the E_{2g} phonon. Insets show temperature (b) and field (c) dependences of the $2\Delta_L^E$ SC coherence peak.

We study the effect of magnetic field on the superconductivity induced spectral features. The intensity threshold $2\Delta_0$ and the $2\Delta_S^E$ features smear out already at magnetic field as weak as 0.2 T, consistent with H_{c2}^{π} deducted from vortex imaging [2]. The $2\Delta^A$ SC coherence peak persists up to 0.6 T while the $2\Delta_L^E$ peak is suppressed only beyond 2 T. $2\Delta_L^E(T, H)$ are shown in the insets of Fig. 2, it exhibits BCS-like temperature dependence and a linear reduction in field with an anomalously rapid slope about -15 cm⁻¹/T. A linear continuation for the $2\Delta_L^E$ gap collapse approximates to 7 T, field higher than $H_{c2}^{optical}$ [3].

In Fig. 2 we summarize temperature dependence of the E_{2g} Raman response for MgB₂ crystal measured on cooling in zero- and 7 T field and as function of field at 8 K. We fit the data with a model containing two phononic oscillators on electronic Raman continuum including the coherence peak in the SC state. The temperature and field dependences of the E_{2g} phonon frequency $\omega(T, H)$ and the damping constant $\Gamma(T, H)$ are shown in panels (c-d).

Following Refs. [7, 8] we relate the electron phonon coupling constant λ to $\kappa = (\omega_0^{SC}/\omega_0^N) - 1$ as $\lambda = -\kappa(T) \Re(\frac{\sin u}{u})$, where $u \equiv \pi + 2i\cosh^{-1}(\omega^N/2\Delta_L^E)$. Using $2\Delta_L^E = 110 \text{ cm}^{-1}$ we estimate λ at about 0.3.

In summary, we have measured the polarization, excitation, temperature and field dependence of the Raman response for MgB₂ single crystal superconductor and observed four distinct superconductivity induced features: (1) a clean gap below 35 cm⁻¹ consistent with the SC gap in π -states of the boron p_z orbitals; (2) a shoulder at 50 cm⁻¹ in E_{2g} spectra; (3) a SC coherence peak of A_{1g} symmetry at 75 cm⁻¹; and (4) the largest gap in E_{2g} spectra at 110 cm⁻¹ consistent with the SC gap in σ bonding states of the boron $p_{x,y}$ orbitals. The features (1-3) are shown to be fragile to magnetic field applied along the *c*-axis. The largest gap (4) shows BCS-like temperature dependence and $2\Delta_L^E/k_BT_c$ ratio about 4 indicating a moderately strong coupling limit. While the $2\Delta_L^E$ coherence peak intensity sustains up to 2 T field the gap magnitude is suppressed at very rapid rate of $-15 \text{ cm}^{-1}/\text{T}$. We study temperature dependence of the E_{2g} boron stretching phonon and conclude that the anharmonic decay is primarily responsible for the anomalously large damping constant of this mode. For this phonon we observe superconductivity induced self-energy effects from which we estimate the electron-phonon coupling $\lambda \approx 0.3$.

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