INTERBAND SCATTERING IN MgB$_2$


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Abstract
The scattering process responsible for connecting the bands remains one of the last open questions on the physical properties of MgB$_2$. Through the analysis of the equilibrium and photo-induced far-infrared properties as well as electron spin resonance of MgB$_2$ we propose a phonon mediated energy transfer process between the bands based on the coupling of quasiparticles to an $E_{2g}$ phonon.

Keywords: MgB$_2$, infrared, ESR, pump-probe, interband scattering

1. Introduction

The discovery of superconductivity in MgB$_2$ [1] triggered a major theoretical and experimental effort to understand its mechanisms. Kortus et al. [2] predicted that that MgB$_2$ should have two metallic bands at the Fermi energy one two dimensional ($\sigma$) band along the $\Gamma$–$A$ direction and another three dimensional ($\pi$) band covering most of the Brillouin zone volume. They also predicted that both bands should undergo the superconducting transition with different energy gaps, the higher being in the $\sigma$ band. Several experimental studies have found evidence for a double gap in MgB$_2$ [3, 4]. In particular Giubileo et al. [3] showed that these two gaps close at the same $T_c$. The first attempt to describe a two band superconductor was done as early as 1959 [5], when Suhi et al. proposed that when two superconducting bands interact the critical temperature ($T_c$) of the lowest gap band increases and joins the one of the highest gap band. This is qualitatively the effect observed in STM measurements. Most of the physics behind superconductivity of MgB$_2$ is not understood [6] and the remaining big question concerns the process responsible for connecting the two bands.
In this work we address this issue by looking at the far-infrared equilibrium and photo-induced reflectivity of a MgB\textsubscript{2} thin film and at the Electron Spin Resonance (ESR) of powder samples.

2. Experimental

Optical data was taken on a $\sim$ 30 nm thick c-axis oriented film of MgB\textsubscript{2} deposited on a sapphire substrate at Postech [7]. Its $T_c$ of 30 K is suppressed compared to the bulk material ($T_c = 39$ K). Standard reflectance measurements were performed using the Bruker 66v FTIR spectrometer at beamline U10A of the NSLS, with synchrotron radiation as the IR source. The specimen was solidly clamped with indium gaskets to the copper cold-finger of a heli-tran cryostat, leaving a 3 mm diameter aperture exposed for the IR measurement. The remaining 80\% of the sample’s surface was available for thermal conduction into the cold finger.

Transient far-infrared photo-reflectance measurements were also performed using the same spectrometer and beamline. Here, we measured the reflectance change due to illuminating the MgB\textsubscript{2} film with 2 ps near-infrared ($\lambda = 760$ nm) pulses from a Ti:sapphire laser. The laser pulses break pairs and weaken the superconducting state for a brief amount of time ($\sim$ 1 ns) [8]. The resulting change in reflectance is sensed with the $\sim$ 1 ns infrared pulses from the synchrotron in a pump-probe configuration [9]. The average laser power was 20 to 50 mW (0.4 to 1 nJ per pulse) so that the MgB\textsubscript{2} film could be maintained at $T = 5$ K. The pulse repetition frequency was 53 MHz, matching the pulsed IR output from the synchrotron. For time-dependent studies, the broadband probe pulses were not spectrally resolved, and the response is an average of the reflectance across the 10 to 100 cm\textsuperscript{-1} spectral range.

ESR data was collected between 40 K and 600 K with a Bruker ESP300E 10 GHz spectrometer equiped with an Oxford ESR He cryostat on MgB\textsubscript{2} powder samples synthesized in Princeton. The powder was mechanically ground to avoid skin depth problems.

3. Results and Discussion

Figure 1(a) shows the ratio of superconducting to normal far-infrared reflectance at equilibrium. The dashed line is a Mattis-Bardeen fit [10] assuming a gap at 43 cm\textsuperscript{-1}. The solid line is obtained using a simple non-interacting carrier model for the conductivity $\sigma = (1 - f)\sigma_\sigma + f\sigma_\pi$ where $\sigma_\sigma$ and $\sigma_\pi$ are Mattis-Bardeen conductivities for each band and $f$ is the fraction of the \pi band that contributes to the total conductivity. The parameters used for the latter are $2\Delta_\sigma = 56$ cm\textsuperscript{-1} and $2\Delta_\pi = 30$ cm\textsuperscript{-1} ($f = 0.6$). Although the 2 gap model better describes the data at low frequencies, the improvement is not sufficient to conclude that two gaps must exist. In fact, previous data on equilibrium
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![Figure 1](image_url)

Figure 1. (a) Equilibrium infrared reflectivity of MgB$_2$ film at 5 K (dots). The lines are fits using the Mattis-Bardeen optical conductivity for systems with one or two gaps. (b) Photo-induced reflectivity of MgB$_2$ film at 5 K (dots). The lines are attempts to describe the data using the same parameters as those from panel (a). The dashed line assumes a single gap. The dotted and continuous lines are calculations for a two gap system. For the former we assume that in the photo-excited state both bands have excess quasiparticles and for the latter, we assume that all excess quasiparticles find themselves in the lower energy gap band ($\pi$). The inset in panel (b) shows the time dependence of the integrated photo-induced signal.

infrared spectra of MgB$_2$ [11] did not provide any clear cut picture about the presence of two bands in MgB$_2$, either. However, the data does not seem to follow strictly the BCS theory.

An analysis of the time dependent transient photo-reflectance gives us a good estimate of the effective pair recombination rate [8]. The inset in Fig. 1(b) shows the average reflectance change as a function of the delay between pump and probe pulses at 6 K. In accordance with other BCS superconductors the effective recombination time is found to be a few nanoseconds. One important remark is that, within the experimental time resolution, no evidence of multiple decays is found. In fact, ultra-fast pump-probe measurements on MgB$_2$ [12, 13] did not find any evidence for a double relaxation down to the ps regime.

Panel (b) in Fig. 1 shows the photo-induced spectra taken with pump and probe at coincidence. The pairs broken by the laser pulse will create an excess quasiparticle population. Owen and Scalapino [14] showed that this excess quasiparticle population weakens the superconducting state. This weakened state can be spectroscopically detected and resolved as a slightly reduced energy gap allowing the transient photo-reflectance data to be analyzed using the same expressions as those for the equilibrium reflectance. The dashed curve in Fig. 1(b) assumes that the system has a single gap at 43 cm$^{-1}$ which is decreased by photo-excitation. Although the amplitude and overall shape of the signal can be reproduced by this simulation, quantitative agreement is not achieved. The dotted line assumes that the system has the same two gaps used in the equilibrium reflectance fit and that in the photo-excited state both gaps
Figure 2. (a) ESR signal for MgB$_2$ at 151 K (circles) and 465 K (triangles). The solid line are fits with an asymmetric Dysonian line. (b) ESR line widths for this work (circles), Ref. [17]. (diamonds) and Ref. [18] (stars). The solid line is the resistivity (normalized to compare with the ESR data) from Ref. [19].

ESR spectroscopy uses a static magnetic field to lift spin states degeneracies by a Zeeman splitting and probes the magnetic dipole transitions between these states with a small perpendicular rf magnetic field. In metals, the high collision rate of quasi-particles defines a single spin-lattice relaxation time $\tau_s$. The electronic spin-orbit interaction has two consequences on the ESR response: (i) a “static” interaction produces a shift in the $g$ factor from the free electron value and (ii) in the presence of phonons a “dynamic” (time averaged) interaction leads to the Elliott-Yafet relation [15]. The Elliott-Yafet relation states that $(\delta g)^2\tau_c/\tau_s = \text{const}$, where $\tau_c$ is the electronic collision scattering time. In a simple one band model these two relaxation rates are proportional, a fact that has been observed in many metals [16].

Figure 2(b) compares the thermal evolution of the MgB$_2$ ESR linewidth (this work and Refs. [17, 18]) with its dc resistivity extract from Ref. [19]. The linewidth is measuring the spin scattering rate and the resistivity gives the physical collison rate.
Interband scattering in MgB$_2$ electron collision rate. Had Elliott-Yafet been followed, the ESR data should agree with the resistivity. Both quantities agree at low temperatures but this agreement breaks down around room temperature. Formally this implies a $g$ factor unexpectedly varying with temperature. However, if one considers that the $\sigma$ and $\pi$ bands have different $g$ factors, a temperature dependent mixing of these bands leads to a temperature dependent effective $g$.

4. **Interband scattering**

The photo-induced spectra in the superconducting state and the ESR data in the normal state can be understood in terms of an interband scattering process. When talking about interband scattering, one may think in terms of transfer of quasiparticles or, alternatively, transfer of the energy of quasiparticles. The latter process can be viewed as a process in which excited quasiparticles in one band relax emitting phonons which can excite quasiparticles in the other band. There is no transfer of the actual quasiparticles but rather of their energy.

The recent inelastic X-ray scattering data of Shukla et al. [20] shows that the $E_{2g}$ phonon at around 60 meV is anomalously large in the $\Gamma - A$ direction of the Brillouin zone, the same direction as the $\sigma$ bands. This $E_{2g}$ phonon is the only phonon showing a large linewidth and it is natural to assume that this effect is coming from a strong coupling with $\sigma$ quasiparticles. However, once created, $E_{2g}$ phonons can scatter quasiparticles in both bands. As the $\pi$ bands occupy a larger volume of the Brillouin zone, it is natural to assume that more quasiparticles in this band will get excited.

This picture naturally explains our data. The photo excited spectra originates from quasiparticles created by a 1.5 eV laser excitation. When quickly relaxing from high energies, the quasiparticles in the $\sigma$ band eventually reach energies comparable with that of the $E_{2g}$ phonon. At that time their energy is transfered to the $\pi$ bands leading to a photo-excited state (at our ns time resolution) that is composed mostly of excess quasiparticles in the $\pi$ band. The ESR response can be understood in similar terms. In this case we have no excited quasiparticles. At lower temperatures the $g$ factor is a mixture of $\sigma$ and $\pi$ bands. When we raise the temperature we give enough energy to the quasiparticles to interact with the $E_{2g}$ phonon. Eventually, this changes the balance between $\sigma$ and $\pi$ bands populations inducing a change in the effective $g$ factor.

5. **Summary**

We looked at the far-infrared equilibrium and photo-induced reflectivity of a MgB$_2$ thin film and at the ESR spectra of powder samples. The photo-induced response shows one gap at 3 meV and another at 7 meV. However, excess quasiparticles are only found at the edge of the smaller gap. ESR data on the normal state shows a break down, around room temperature, of the
Elliott-Yafet time relaxation behavior observed in virtually any metal. These effects can be described in terms of an interband energy transfer process mediated by the anomalously broadened $E_{2g}$ phonon [20].

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References