Inelastic X-ray scattering and first-principles study of electron excitations in MgB$_2$

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Abstract
An experimental and theoretical study of electronic excitations in MgB$_2$ covering the domain of large energy and momentum transfers is reported. Energy-loss spectra for several values of momentum transfers were measured in a polycrystalline sample by means of inelastic X-ray scattering spectroscopy. Ab initio calculations of the dielectric function as well as the energy-loss function were performed in the frame of the time-dependent local density approximation within inclusion of crystal local-field effects. We obtained very good agreement between the experimental and the theoretical energy dispersion of the peak maximum of the loss function. We found that crystal local-field effects are responsible for this agreement at large momenta. Fine structure observed in the measured spectra was interpreted in terms of strong interband transitions predicted by the calculations in the $\Gamma A$ and $\Gamma K$ directions. The theoretical dispersion of these features is in good accordance with the experimental data. Further spectral features in the measured spectra due to Mg 2s and 2p core electron excitations are also discussed.

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Soon after the discovery of superconductivity at $\sim$ 39 K in magnesium diboride [1], much theoretical effort was devoted to studying collective electron excitations in this compound [2–4]. Those investigations were based on first-principles calculations of the frequency- and momentum-dependent density-response function. Besides the expected free-electron-like plasmon at $\sim$ 20 eV, a long-lived plasmon mode at lower energies was predicted. This novel collective mode was ascribed to strong coherent charge fluctuations between parallel Mg and B sheets. High resolution inelastic X-ray scattering measurements at low momentum transfers ($q < 0.77$ a.u.) [5] allowed the predicted energy dispersion and anisotropy of both plasmon modes to be experimentally verified. Later on [6], using the same experimental technique but with improved energy resolution, the low-energy collective excitation was demonstrated to exist not only for small $q$, but to reappear periodically in higher Brillouin zones (BZ) at energies between 2.5 eV and 4.5 eV. This novel charge excitation embodies a unique signature of the layered electronic structure of MgB$_2$. Very recently, the first-principles calculations [7,8] demonstrated that long-lived plasmon modes corresponding to charge density fluctuations between carriers in $\sigma$ and $\pi$ boron bands should exist at energies below 0.5 eV, where they might strongly interact with lattice vibrations.

The cross section for an inelastic X-ray scattering process is directly related to the imaginary part of the inverse dielectric function $\epsilon^{-1}(q, \omega)$, the so-called energy-loss function (ELF) [9], $-\text{Im}[\epsilon^{-1}(q, \omega)]$, which reveals information about the scattering electron system concerning its energy ($\omega$) and momentum ($q$) transfer-dependent response to an external perturbation. Due to the negligible contribution of multiple scattering processes, which means a negligible distortion of the X-ray energy-loss spectra, as
well as to the enhanced cross section at high momentum transfers, inelastic X-ray scattering spectroscopy (IXSS) has become a well-suited technique to investigate both valence and core electron excitations [9]. IXSS is particularly appropriated in the range of intermediate and high momentum transfers, where electron energy-loss spectroscopy (EELS) could be hardly applied. In addition, due to the large penetration depth of hard X-rays, IXSS yields true bulk information and is not sensitive to contamination or radiation damage of the sample surface. In this work we extend the range of both energy and momentum transfers covered in previous experimental and theoretical studies, using inelastic X-ray scattering spectroscopy and first-principles calculations of the density-response matrix within the framework of the time-dependent density functional theory [10–12].

Inelastic X-ray scattering experiments were performed on the D12A-XRD1 beamline at the National Synchrotron Light Laboratory (NLNS). The synchrotron white beam was monochromatized by means of a sagittally focusing, Si(111) double-crystal monochromator. A bent X-ray mirror placed upstream of the monochromator was operated in parallel-beam configuration so as to reduce the natural synchrotron beam divergence and thus to reduce the energy bandwidth of the beam transmitted by the monochromator. Energy analysis of the scattered photons was accomplished by utilizing a focusing nearly backdiffracting (89.2 °) Be(110) silicon crystal, in four-crystal geometry, using the Si(333) reflection. Further details about the experimental setup can be found elsewhere [13]. Measurements were performed at room temperature and in vacuum. Energy-loss spectra were recorded for a wide range of momentum transfers, going from 0.55 a.u. to 2.4 a.u. The overall energy resolution of the spectrometer as determined from the FWHM of the elastic lines was 1.07 eV at 5.93 keV incident photon energy. Annular diaphragms of 2.4 a.u. angular aperture were placed in front of the analyzer. This type of diaphragms allowed the transferred momentum resolution to be improved without largely diminishing the collected solid angle, as demonstrated in a previous work [14]. The overall transferred momentum resolution (FWHM) ranged from 0.066 a.u. (q = 0.55 a.u.) to 0.044 a.u. (q = 2.4 a.u.). Depending on the scattering angle, between 2 × 10^4 and 6 × 10^4 counts were collected in a single measuring point at the maximum of the inelastic peak.

The polycrystalline MgB$_2$ samples studied were prepared by a solid-state reaction method. Elemental Mg (99.9% pure) and boron powder (99.9% pure) were combined in the stoichiometric ratio. The mixture was put inside a Ta tube and sealed in an argon atmosphere. The Ta tube is then sealed inside a quartz tube in a vacuum atmosphere. Finally, the system was placed in the furnace and heated slowly up to 950 °C and kept at this temperature for 2 h, and then removed and placed into liquid nitrogen to cool it to room temperature. The sample was characterized by magnetic susceptibility and X-ray powder diffraction measurements. dc-Magnetic susceptibility measurements showed the superconducting transition temperature in $T_c \approx 39$ K, in good agreement with literature [1], while X-ray diffraction indicated a minor MgO impurity phase ($\approx$4%). The polycrystalline pellets had a diameter of 10 mm and were about 1 mm (reflection geometry) and 0.075 mm (transmission geometry) thick.

X-ray energy-loss scans at different momentum transfers are presented in Fig. 1. The spectra were normalized to the monitor signal and a constant background, as that determined from the energy-gain side of the elastic line, was subtracted. Fig. 1 shows that a nearly Lorentzian-shaped peak extends up to $q = 0.8$ a.u., in agreement with a previous IXSS-study [5]. This peak resembles a free-electron-like plasmon resonance (occurring at 19.2 eV for $r_1 = 1.82$, corresponding to eight bound electrons in the unit cell of MgB$_2$), disperses positively and broadens with increasing $q$. The magnitude of the plasmon cut-off vector for the corresponding free electron gas is $q_e = 0.74$ a.u. Above 0.8 a.u., the lineshape becomes distorted and broadens rapidly as the momentum transfer increases, and some fine structure begins to arise in the energy-loss spectra.

We start the calculations from the evaluation of a set of eigenfunctions $\psi_{n,k}(\mathbf{r})$ and eigenvalues $e_{n,k}$ of the self-consistent Kohn–Sham equation of density-functional theory. In the calculations, the experimental parameters $a = 5.8317$ a.u. and $c = 6.6594$ a.u. of the hexagonal lattice of MgB$_2$ were used. The wave functions $\psi_{n,k}(\mathbf{r})$ were expanded in a plane-wave basis with a kinetic-energy cutoff of 24 Ry and the exchange–correlation potential $V_{xc}$ was taken in the form of Ref. [15]. Interaction of valence electrons with the Mg and B ions was described by non-local norm-conserving pseudopotentials [16].

At the next step we evaluate a spectral function $S^0_{\mathbf{G}G}(\mathbf{q}, \omega)$ as follows [17]:

$$S^0_{\mathbf{G}G}(\mathbf{q}, \omega) = \frac{2}{\Omega} \sum_{k}^{\mathbf{BZ}} \sum_{\mathbf{n}}^{\text{occ}} \sum_{\mathbf{n'}}^{\text{unocc}} \langle \psi_{n,k}\rangle \langle e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} | \psi_{n',k+\mathbf{q}} \rangle \times \langle \psi_{n'\mathbf{k+q}} | e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} | \psi_{n\mathbf{k}} \rangle \delta(e_{n,k} - e_{n',\mathbf{k+q}} + \omega),$$

where $\mathbf{BZ}$ is the Brillouin zone. Through the equations $\mathbf{G}_{\mathbf{G}}(\mathbf{q}, \omega) | \mathbf{G}_{\mathbf{G}}(\mathbf{q}, \omega) \rangle = \frac{1}{\pi} \text{sgn}(\omega) \text{Im} \chi_{\mathbf{G}G}(\mathbf{q}, \omega)$. In Eq. (1) the factor 2 accounts for the spin, $n$ and $n'$ are the band indices for occupied and unoccupied states respectively and in the sum over $\mathbf{k}$ in the first BZ a mesh including $108 \times 108 \times 80$ points was used. In numerical calculations of $S^0_{\mathbf{G}G}(\mathbf{q}, \omega)$ the delta function $\delta$ in Eq. (1) was replaced by a Gaussian with broadening parameter of 0.1 eV. In the Fourier expansion 25 reciprocal-lattice vectors $\mathbf{G}$ were employed. The real part of the $\chi_{\mathbf{G}G}$ matrix elements is evaluated via the Hilbert transform. Subsequently, the energy-loss function $\text{Im} \epsilon(\mathbf{q}, \omega) = -\text{Im} \epsilon^{\mathbf{q}}(\mathbf{q} + \mathbf{q}, \omega)$ for a given momentum $\mathbf{q} + \mathbf{G}$ (where $\mathbf{q}$ is confined to the first BZ) is obtained from the density-response function $\chi_{\mathbf{G}G}(\mathbf{q}, \omega)$ of an interacting electron system as

$$\epsilon_{\mathbf{G}G}^{-1}(\mathbf{q}, \omega) = \delta_{\mathbf{G}G} + \nu_{\mathbf{G}G} \chi_{\mathbf{G}G}(\mathbf{q}, \omega),$$

which, in turn, is related to $\chi^0$ via the matrix equation

$$\chi_{\mathbf{G}G}(\mathbf{q}, \omega) = \chi^0_{\mathbf{G}G}(\mathbf{q}, \omega) + \sum_{\mathbf{G}_1,\mathbf{G}_2} \chi^0_{\mathbf{G}_1G_2}(\mathbf{q}, \omega) \times [\nu_{\mathbf{G}_1G_2} \delta_{\mathbf{G}_1G_2} + K_{\mathbf{G}_1G_2}(\epsilon_{\mathbf{G}G}(\mathbf{q}, \omega))] \chi_{\mathbf{G}_1G_2}(\mathbf{q}, \omega).$$

Here, $\nu_{\mathbf{G}G}$ is the Fourier transform of the bare Coulomb potential, and $K_{\mathbf{G}_1G_2}(\epsilon_{\mathbf{G}G}(\mathbf{q}, \omega))$ are the Fourier coefficients of the functional derivative of the exchange–correlation potential, which within adiabatic local-density approximation (ALDA) [18] (used in present work) is expressed as

$$K_{\mathbf{G}_1G_2}(\epsilon_{\mathbf{G}G}(\mathbf{q}, \omega)) = \int d\mathbf{r} e^{-i(\mathbf{G}_1 - \mathbf{G}_2)\cdot\mathbf{r}} \frac{d\nu_{\mathbf{G}G}(\epsilon_{\mathbf{G}G}(\mathbf{r}))}{d\epsilon_{\mathbf{G}G}(\mathbf{r})}.$$

The calculated energy-loss functions, along with the real and imaginary part of the dielectric function, are displayed in Fig. 2 for $\mathbf{q}$ along $\Gamma K$ and $\Gamma A$ directions. A marked anisotropy in the shape of $\text{Im} \epsilon^{\mathbf{q}}(\mathbf{q}, \omega)$ can be clearly observed. At low $q$-values, the loss function for $\mathbf{q} | \Gamma K$ consists mainly of a single peak, corresponding to the free-electron-like plasmon submode in the hexagonal plane, whereas for $\mathbf{q} | \Gamma A$ a double-peak structure is exhibited. Also the weaker low-energy plasmon peak is clearly seen below 5 eV. This anisotropy in the shape of the loss function was observed at intermediate and low momentum transfers in the previous IXSS measurements performed on a single-crystal MgB$_2$ sample [5]. In the double-peak structure for $\mathbf{q} | \Gamma A$, the first peak ($\approx 19$ eV) corresponds to the free-electron-like plasmon submode along the
c-axis, while the peak at higher energies ($\sim$25 eV) is associated with an interband transition. As $q$ increases, the overall shape of the theoretical energy-loss functions changes severely and further spectral features appear. As pointed out in Ref. [2], it is difficult to find out which interband transitions are responsible for the peaks in the ELF, because many bands are involved when high-energy and momentum excitations take place.

Fig. 3 shows the dispersion of the peak maximum and the spectral features observed in the experimental energy-loss spectra along with the results of the present calculations. The energy position of the peaks (shoulders) were determined by inspecting the zero crossing points of the first (second) derivatives. From $q = 0.55$ a.u. to $q = 0.8$ a.u., the direction-averaged plasmon, as measured in a polycrystalline sample, disperses almost linearly and its energy is close to the energy of the free-electron-like plasmon along the $\Gamma K$ direction (see Fig. 2). The calculations of the ELF made for $q \parallel \Gamma M$ have shown that the plasmon dispersion is nearly isotropic in the hexagonal plane. The plasmon peak for $q \parallel c$-axis lies at lower energies ($\sim$19 eV, weakly dispersing at low momentum transfers) and is less intense than that for the $q \parallel c$-axis, as is seen in Fig. 2. The excitation spectra in polycrystalline MgB$_2$ for $q \lesssim 0.8$ a.u. are therefore dominated by collective excitations in the hexagonal plane. The calculations of the loss function were carried out with and without inclusion of crystal local-field effects (CLFE) [19,20]. While the agreement between the experiment and theory including CLFE is very good, except only at $q = 0.55$ a.u. where a small difference exists, the dispersion of the peak maximum of the ELF without CLFE separates systematically from the experimental data as $q$ is increased. The important role played by CLFE in the low-energy charge–excitation spectra of MgB$_2$ at large momenta was recently demonstrated by Cai et al. [6] and Silkin et al. [7]. They showed that large CLFE mediate the strong coupling between single-particle and collective excitation channels, leading to striking periodic cosine-like [6] and sine-like [7] energy dispersion of the low-energy plasmons as $q$ goes through successive BZs along the $\Gamma A$ direction. On the other hand, CLFE were found to be negligible in the range of small momentum transfers [2]. Present experimental dispersion is also in very good agreement with the results obtained by Galambosi et al. [5].

A weak but, in a detailed inspection, noticeable splitting into a double-peak shape is exhibited by the main loss peak of the polycrystalline spectra between $q = 0.93$ a.u. and $q = 1.06$ a.u. The low-energy peak (B) corresponds to the continuation of the plasmon submode in the hexagonal plane, whereas the peak at higher energy (C) can be related to an interband transition giving rise to the intense peak at the high-energy side (peak dispersing between 25–28 eV in Fig. 2 for $q \parallel \Gamma A$) of the $\Gamma A$-plasmon. The peak C appears in the calculated ELF of Ref. [2] at momenta as low as $\sim$0.1 a.u., and was also observed by Galambosi et al. [5] in a single-crystal sample for $q \parallel c$-axis and 0.4 a.u. $< q < 0.77$ a.u. We observed in present theoretical ELF that this peak gains intensity as $q$ increases and reaches a maximum at $\sim$0.7 a.u. At this $q$-value its intensity is comparable to that of the collective excitation peak. Above 0.7 a.u., the peak loses intensity and becomes narrower. At higher momentum transfers ($q \sim 1.2$ a.u.) this feature is still noticeable in the calculated ELF, however it is not strong enough to be resolved in the polycrystalline spectra. As Fig. 3 shows, the theoretical dispersion of this feature is in good agreement with the present and previous [5] experimental data. Zhukov et al. [2] also performed calculations of the dielectric function and the ELF.

Fig. 1. Experimental X-ray energy-loss spectra of polycrystalline MgB$_2$ as a function of the transferred energy for different magnitudes of momentum transfer (left: 0.55 a.u. $\leq q \leq 1.06$ a.u.; right: 1.20 a.u. $\leq q \leq 2.4$ a.u.). The spectra are vertically displaced for clarity. Error bars due to counting statistic are shown at around the spectrum maximum. Elastic lines are not shown in the spectra.
Fig. 2. Theoretical energy-loss function for some selected $q$-values, for $q\parallel \Gamma K$ (left) and for $q\parallel \Gamma A$ (right). In the inset, the real (dashed line) and imaginary (solid line) parts of the corresponding dielectric function are shown. Calculations include crystal local-field effects.

Fig. 3. Experimental and theoretical dispersions of the main peak of the energy-loss function and of some spectral features.

For a hypothetical crystal structure $B_2$, obtained from the MgB$_2$ lattice by removing the Mg atoms. Though in general the band-structures and the shape of the loss functions of MgB$_2$ and $B_2$ are quite similar, the feature at the high-energy side of the $\Gamma A$-plasmon is not present in the loss function of $B_2$ [2]. This double-peak structure seems thus to be a signature of the MgB$_2$ crystal.

For $q = 0.93$ a.u. and $q = 1.06$ a.u., two weak structures appearing as shoulders in the high-energy tail of the measured energy-loss spectra (features D and E) can be resolved. These structures can be ascribed to interband transitions, which show up as strong peaks in the calculated ELF, as shown in Fig. 2 at $\sim 30$ eV for $q\parallel \Gamma A$ ($q = 0.919$ a.u.) and at $\sim 33$ eV for $q\parallel \Gamma K$ ($q = 0.937$ a.u.). The interband feature for $q\parallel \Gamma K$ was observed in the theoretical ELF from $q = 0.8$ a.u. to $q = 1.44$ a.u., whereas for $q\parallel \Gamma A$ it is confined to a smaller $q$-range. The dispersion of these features is shown in Fig. 3. The agreement between the experimental and theoretical values is fairly good. The calculations of the ELF for $q\parallel \Gamma M$ have not revealed the pronounced peak predicted for $q\parallel \Gamma K$. This could be a sign of some anisotropy in the electron excitation spectra in the hexagonal plane of MgB$_2$ [8]. The shoulder at $\sim 20$ eV (A) is originated by the $\Gamma A$-plasmon submode.

Since the cross section for inelastic X-ray scattering by inner-shell electrons depends on the magnitude of the momentum transfer as $q^2$ in the dipole approximation [21], features due to core electron excitations are expected to be enhanced as $q$ is increased. At momentum transfers higher than 1 a.u., some spectral features above 50 eV (marked as F to J in Fig. 1) can be identified, despite
the underlying high-energy tail of the strong electron–hole pair excitation spectra. As no remarkable features can be distinguished at high energies in the calculated ELF for valence electrons, all observed fine structures in the high-energy region should be attributed to the core electron excitations. For the Mg 2p core-level energy in MgB$_2$, different experimental values ranging from 49.35 eV to 51.7 eV have been reported in the literature [22–28]. The onset of Mg 2p transitions can be noticed by the appearance of the structure F at $\sim$50 eV. The weak structure at $\sim$55 eV ([G]) can be related to a strong resonance of the Mg $L_{2,3}$ edge in MgB$_2$ observed also in EELS measurements [29]. Jiang et al. [29] suggested that this feature should be originated by an exciton-like transition. Based on the real-space multiple scattering approach (RSMS), calculations of the unoccupied density of states (DOS) in MgB$_2$, accounting for core-hole effects in the final state, were performed in Ref. [29]. According to these calculations, the excitonic state should be coupled to a peak in the empty Mg 3s DOS located $\sim$5 eV above the Fermi level, and within the 5 eV wide pseudogap of the B $\sigma$ states. X-ray absorption studies at the Mg 2p core level in MgB$_2$ by Kurmaev et al. [24] revealed a pronounced structure in the absorption spectra at $\sim$54 eV, in close agreement with present IXSS and previous EELS [29] data. According to theoretical band structure studies [30,31], Mg is well described as being doubly ionized in the compound MgB$_2$. Transitions of 2p electrons of Mg$^{++}$ to excitonic states were also observed in highly ionic compounds as Mg halides [32,33] and MgO [34,35] at around 54 eV.

For q $\geq$ 1.44 a.u., a broad shoulder structure around 72 eV (H) is identified in the experimental spectra. The origin of this structure can be ascribed by arising from dipole-allowed transitions of Mg 2p electrons into unoccupied Mg states of d symmetry. RSMS calculations of the symmetry-projected DOS in MgB$_2$, including effects of the 2p core-hole, revealed a prominent peak in the Mg 3d DOS located about 21 eV above the Fermi level [29], in accordance with the relative position of the feature H in present loss spectra. This structure is related to a well-known characteristic feature of the L$_{2,3}$ absorption spectrum of Mg metal [36], which has also been observed in X-ray Raman spectra at the L$_{2,3}$ edge of Mg more recently [37,38]. The measured energy for the Mg 2s core level in MgB$_2$ is 90.1 eV [28]. The structure at $\sim$90 eV (feature I) indicates the onset of Mg 2s transitions. A visible shoulder at 95 eV for q = 2.0 a.u. (feature J) evolves into a prominent peak for q = 2.4 a.u. The calculated magnesium p-DOS in MgB$_2$ exhibits a maximum at $\sim$10 eV above the Fermi level [39]. The inclusion of 1s core-hole effects shifts the empty Mg p-like states 4 eV towards lower energies and increases the density of states compared with the ground state case [39]. Assuming that the 2s core-hole potential is weaker screened than the 1s core-hole, effects of the former on the empty DOS are expected to be even stronger, shifting the features of the p-DOS even closer to the Fermi level. One could therefore attribute the feature at 95 eV to dispole-allowed transitions from Mg 2s-states to empty p-symmetry final states. It should be noted that the structure showing up at the onset of transitions from the Mg 2p core level (feature F) gains spectral weight as q increases, evolves to a pronounced peak for q $\approx$ 1.75 a.u., and then vanishes at higher momenta. Based on calculations of the symmetry-projected Mg empty DOS alone, an explanation of the behavior of the peak F cannot be given. In the range of high q values investigated in this work it is q $\gg$ $\alpha$ $^{-1}$, $\alpha$ being the electron orbital radius for the Mg 2s or 2p level. Thus, the dipole limit (q $\ll$ 1) is no longer valid and dipole forbidden transitions may start to contribute significantly to the scattering cross section. The rapid increase of the spectral weight of some features could be attributed to monopolar excitations channels, coming into play as q is increased. In order to elucidate the evolution of the loss features by core electron excitation for increasing q, first-principles calculations of the X-ray Raman scattering cross section accounting for the q and energy dependence of the matrix elements and including core-hole effects in the final states, as performed by Soininen et al. [40] using a generalization of the RSMS approach, are required.

In summary, we report new measurements and calculations of the energy-loss spectra of MgB$_2$ in a wide range of energy and momentum transfers. Both high energy and high momentum-transfer resolution were essential to be able to resolve fine structures in the X-ray energy-loss spectra of a polycrystalline sample. Major features observed in the experimental spectra were interpreted in terms of ALDA-based calculations of the loss function. The very good agreement between experiment and theory shown by the dispersion of the peak maximum revealed the need for accounting for crystal local-field effects in the calculations, when high q values are involved. On the basis of the present calculations, the q-dependent fine structure observed in the domain of valence electron excitations can be traced back to features originated from interband transitions for q along ΓK and ΓA directions. A good agreement was obtained between the theoretical and experimental dispersion of the spectral features. Some small existing discrepancies can be caused by imprecisions in determining the energy position of the features in polycrystalline spectra. Some fine structures appearing in the domain of Mg 2s and 2p electron excitations were discussed in terms of the unoccupied Mg DOS in MgB$_2$. Further IXSS-experiments in a single crystal sample would be needed in order to carry out more precise investigations on the direction-dependent rich fine structure exhibited by the electron excitation spectra of this superconducting system.

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