Out-of-equilibrium electronic dynamics of the transition metal dichalcogenides $MoTe_2$ and WTe_2

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Introduction

The discovery of topological insulators (TIs) stimulated, on one side, the classification of the topological phases of matter; on the other side it fuelled the synthesis and the characterization of new materials [1]. Among these, Weyl semimetals (WSMs) have attracted considerable attention, since they host exotic particles, the chiral Weyl fermions, which have been only predicted by theory in high-energy physics [2, 3].

Condensed matter physics has become playground for the search of particles those are not constrained by Poincare symmetry [4] or Lorentz invariance, such as the so-called type-II Weyl fermions [5]. Their distinctive trait is a tilted Weyl cone, emerging at the touching point of the valence (VB) band and conduction band (CB). WTe_2 and $MoTe_2$ [6] have been recently proposed to realize this type-II WSM phase, although the experimental confirmation is still lacking for the first compound [7, 8]. Whereas, the complex low-temperature band structure of $MoTe_2$, characterized by both trivial arc [9] and topological Fermi arc [10, 11], has been shown to be compatible only with the type-II WSM phase [11].

What makes $MoTe_2$ even more interesting is the structural phase transition ($T^* = 257$ K) between the low-temperature orthorhombic and the high-temperature monoclinic structures. This transition must, in fact, be accompanied by a change in the material topological nature, since the high-temperature phase is centrosymmetric and cannot host chiral Weyl fermions [2]. Figure1(a) schematizes this topological phase transition (TPT) and the opening of the gap at the Weyl point (WP). However, the presence of a bandgap cannot be directly investigated with conventional ARPES, since the WP is located above the Fermi level (E_F). In our experiment, we have followed a different strategy, by exploiting tr-ARPES to follow the electron dynamics above E_F, comparing the response of $MoTe_2$ in the two topological phases to the one of the sister compound WTe_2.

Results

Figure1(b) shows the band structure of $MoTe_2$ measured at ARTEMIS with 17.5 eV photon energy, along the direction where theory predicts two pairs of WPs to be located, slightly above E_F, at 5 meV and 50 meV [9], respectively. No differences are resolved in the bare band dispersion when crossing the TPT, from 50 K (left) to 300 K (right) [12].

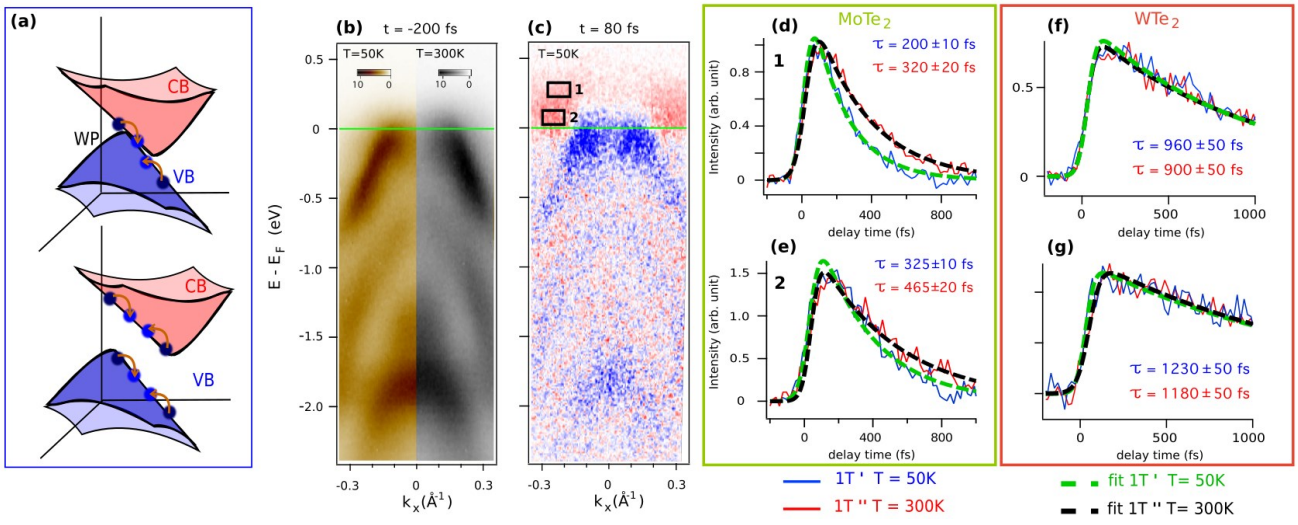

Figure 1 (adapted from Reference [12]): (a) Sketch of the tilted Weyl cones in the WSM phase (top) and the gap opening in the trivial phase (bottom). (b) Measured band dispersion in $MoTe_2$ at 50 K (left) and 300 K (right). (c) Difference between the ARPES image 80 fs after and 200 before optical excitation. (d) - (e) Population dynamics of $MoTe_2$ integrated at 50 K (blue) and 300 K (red) in the area highlighted in panel (c) by the rectangles. (f) – (g) Comparison between the population dynamics measured at 50 K (blue) and 300 K (red) in WTe_2. The best fit and the corresponding characteristic time are shown, as well.

Signatures of the gap opening are resolved in the electron dynamics. Figure1(c) shows the differential image in the WSM phase, obtained as difference between the data 80 fs after and 200 fs before the arrival of the pump pulse, with 2 eV photon energy [12].

Electrons are removed from the VB (blue) and transferred in the unoccupied CB (red), above the WPs. Rectangles highlight the two regions of the band structure where the intensity has been integrated. Figure1(d) – (e) compare the carrier population dynamics, at low- (blue) and high- (red) temperatures. Dashed green and black lines show the best fit obtained with a decaying exponential, whose characteristic relaxation times are shown, as well. The dynamics is found to be 30-50% slower in the high-temperature phase. We attribute this slowdown to the opening of the gap at the WPs in the trivial phase. The bandgap acts as a bottleneck in the relaxation dynamics, as it reduces the phase space available for electron-electron scattering and electron-phonon scattering [12].

In order to further validate our interpretation, and to rule out any possible trivial dependence of the dynamics on the temperature, we investigated also the out-of-equilibrium electronic properties of WTe_2. This material has similar band structure, but it shows no structural transition as a function of temperature, and the WSM is still discussed [7, 8]. Figure 1 (f) – (g) summarize the results of this study, the electron dynamics of WTe_2 is integrated in the same regions previously analyzed for $MoTe_2$. No effect is observed by changing the sample lattice temperature. Moreover, we recognize that the relaxation times, as obtained from the best fit, is approximately three times slower than the one reported in the trivial phase of $MoTe_2$ [12].

This observation indicates that in WTe_2 several scattering mechanisms are forbidden. This is consistent with the existence of a bandgap, as shown by our *ab initi*o calculations [12], with a local direct gap E_g = 8-12 meV, whose value is larger then the lowest energy optical phonons, which cannot contribute to the interband scattering [12].

Conclusions

In conclusions we have compared the electron dynamics in the unoccupied density of states of $MoTe_2$ in the WSM and trivial phases [12]. We have reported a slowing down of the relaxation dynamics in the high-temperature centrosymmetric phase, as a consequence of the gap-opening. We compare this observation to the case of WTe_2, whose topological phase is still debated. The observed longer dynamics is compatible with its topological trivial nature [12].

We show that tr-ARPES can be exploited to probe the consequences of topological order in novel materials.

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