Correlation between electronic and structural orders in 1T-TiSe₂

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The correlation between electronic and crystal structures of 1T-TiSe₂ in the charge-density wave (CDW) state is studied by x-ray diffraction in order to clarify basic properties in the CDW state, transport properties, and chirality. Three families of reflections are used to probe atomic displacements and the orbital asymmetry in Se. Two distinct onset temperatures are found: \(T_{CDW}\) and a lower \(T^*\) indicative for an onset of Se out-of-plane atomic displacements. \(T^*\) coincides with a DC resistivity maximum and the onset of the proposed gyrotropic (chiral) electronic structure. However, no indication for chirality is found. The relation between the atomic displacements and the transport properties is discussed in terms of Ti 3d and Se 4p states that only weakly couple to the CDW order.

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Electron (hole) localizations are central concepts in condensed matter systems and are directly relevant for charge-density wave (CDW) order, exciton formation, and superconductivity. The transition-metal dichalcogenide 1T-TiSe₂ has long been studied due to its wide variety of exciting physical phenomena such as CDW formation [1,2], the possible emergence of a Bose-Einstein condensate [3,4], and, very recently, the observation of a gyrotropic electronic order [5]. Additionally, emergent superconductivity is found in the vicinity of the CDW phase [6–10]. This wide variety of properties suggests complex relations among electronic structure, transport, and the crystal structure [11–17]. Many of these basic properties are only poorly understood despite decades of intensive research on this material. Open points are (1) interplay of electronic and crystal structures below the CDW phase transition temperature \(T_{CDW}\) (≈202 K) and the DC resistivity maxima [1,17], and (2) a possible emergence of chirality in the crystal structure [18–20] or solely in the electronic structure [5,21–25], and its decoupling from the CDW (different onset temperature).

DC resistivity shows an increase at \(T_{CDW}\) which is due to charge localization and gap formation, similar to other CDW systems [26–28]. However, a large and broad peak in the resistivity is seen at a temperature lower than \(T_{CDW} \approx 165 \text{ K}\); see Ref. [1]). It has been suggested that this anomalous peak originates from a crossover between two temperature regimes: from the low-temperature state with negative carriers (electrons) resulting from a small extrinsic doping to a high-temperature state with both negative and positive carriers (electrons and holes) which arise due to thermal fluctuations [17].

Besides the anomalous resistivity peak, the CDW state also features a circular photogalvanic current, measured with midinfrared circularly polarized light irradiation, interpreted as the occurrence of gyrotropic electronic order [5] and the emergence of chirality [18], both of which have distinct onset temperatures below \(T_{CDW}\). The chiral phase transition, as claimed to be observed by scanning tunneling microscopy (STM) and x-ray diffraction (XRD) experiments [18–20], takes place \(\approx 7 \text{ K}\) lower than \(T_{CDW}\) [20]. Such a chiral CDW order is proposed as stacking three one-dimensional CDW layers with different wave vectors to each other in a chiral way [21–25], and is manifested by chiral atomic displacements with \(P1\) symmetry and a possible orbital order. However, these experimental findings have been challenged by alternative...
The electronic and crystal structures and their temperature interpretations [29–31]. It is, therefore, important to clarify the electronic and crystal structures and their temperature dependence.

In this Letter, we study in detail the various structural modifications below $T_{CDW}$ in a thin flake of single-crystalline 1T-TiSe$_2$. The Bragg reflections, which appear in the CDW state, are ascribed to specific atomic motions. The change in transport properties below $T_{CDW}$ is discussed in terms of a possible change of orbital hybridization caused by one of these atomic motions which weakly correlates to the CDW order. Although the onset temperature of certain reflections deviates from $T_{CDW}$, no evidence of chirality [20] is found. Detailed investigations of a space-group forbidden reflection in resonant XRD combined with $ab$ initio simulation are well described by a nonchiral symmetry of electronic and crystal structures in the CDW state.

Moreover, the valence-band maximum at the $\Gamma$ point and the conduction-band minima (normal state $L$ points) are strongly hybridized at the $\Gamma_{CDW}$ point and are significantly repelled from the Fermi energy. A recent photoemission study revealed, however, that a branch of the conduction band derived from Ti 3$d_{z^2}$ states remains as in the normal state, indicating only a weak correlation to the CDW order [35]. This Ti 3$d_{z^2}$ band crosses the Fermi level and dominates transport properties in the CDW state. In contrast, the repulsion of the valence band maximum results in a valence-band maximum of the CDW state that is no longer at the $\Gamma$ point but is located at the $A$ point, at which the states are only weakly affected by the CDW order. The band structures for both the states are schematically drawn in Figs. S1(a) and 1(d) [33].

Both Ti and Se atoms, each of which occupies a single crystallographic site in the normal state ($P\bar{3}m1$), become two distinct sites in the CDW state ($P3c1$), as shown in Figs. 1(a) and 1(b) [32]. While Ti1 and Se2 have only single in-plane ($\delta_{Ti}$) or out-of-plane ($\delta_{Se,\text{out}}$) displacements from the normal state, respectively, Se1 has both types of components ($\delta_{Se,\text{in}}$ and $\delta_{Se,\text{out}}$ in-plane and out-of-plane, respectively). Since there are two Se sites, the out-of-plane motions of these sites are independent and we can define their difference as $\Delta\delta_{Se} = \delta_{Se,\text{in}} - \delta_{Se,\text{out}}$.

A single crystal of 1T-TiSe$_2$ grown by the iodine vapor transport method [35] was cleaved along the (001) plane by repetitive exfoliation, and a flake ($\approx 2$ $\mu$m thickness) was mounted on a polycrystalline diamond substrate. Experiments were performed at the beamline I16 [36] of Diamond Light Source. The sample was mounted on the cold finger of a closed-cycle refrigerator attached to a Newport six-circle kappa diffractometer and cooled down well below $T_{CDW}$ and $T^*$. The photon energies of x-ray beams were tuned to 12.6 keV for nonresonant XRD and around the Se $K$ edge ($\approx 12.658$ keV) for resonant XRD. A Si (111) analyzer was used to determine the polarization state of the scattered beam. Scattered photons were counted using a PILATUS 100K pixel detector [37] and using an avalanche photodiode during azimuthal scans at resonance. A rocking curve as well as a raw two-dimensional image of (1 0 7) shown in Fig. S2 [33] confirm the high crystalline quality of the sample. An x-ray-absorption spectrum (XAS) was obtained by integrating the fluorescence signal. DC resistivity was measured for a single crystal from the same batch as that used for this XRD study along the (001) plane by the four-point resistance method. The resistivity peak at $T^*$ of our sample is significant as seen in Fig. 2(a), and $T^*$ matches that of a high-quality polycrystalline sample [1].

We classify the measured Bragg reflections into three families, A, B, and C, all of which are space-group forbidden in the normal state. We denote reflections by using the indices in the normal state, $h$, $k$, and $l$. Family A represents ($h$ $k$ $l$) reflections where $l$ and at least one of $h$ or $k$ are half integers. These reflections appear at $G + q$, where $G$ is a reciprocal-lattice vector of the normal state, and thus directly measure the displacement of the lattice from the CDW order. Family B represents the $(0$ $k$ $l)$ type of reflections where $l$ is an integer while $k$ is a half integer. Family C also represents the $(0$ $k$ $l)$ type of reflections but with both $l$ and $k$ as half integers. Note that family C is even space-group forbidden in...
FIG. 2. Integrated intensities of reflections belonging to families A (0.5 1 1.5), B (0 0.5 8), and C (0 0.5 9.5), and DC resistivity as functions of temperature. XRD data shown in (a) [(b)] were acquired at 12.6 keV [the Se K edge]. The DC resistivity is normalized by the data at 300 K. The green, red, and blue solid lines represent power-law fits \( \propto (T_c - T)^\alpha \), where \( T_c \) and \( \alpha \) are the critical temperature and critical exponent, respectively. The black line represents the quartic term with an onset at \( T_{\text{CDW}} \).

the CDW state and is observed only at resonance (as shown later).

Figure 2 shows the temperature dependence of the integrated intensities of the three families together with the DC resistivity. The reflections (0.5 1 1.5) (family A, off resonance) and (0 0.5 9.5) (family C, at resonance) appear at \( T_{\text{CDW}} \) and their intensities grow proportional to the square root of \( T_{\text{CDW}} - T \). Note that the temperature \( T_{\text{CDW}} \) is the same as that of a high-quality polycrystalline sample [1], indicating no significant impurity nor off-stoichiometry of our sample. On the other hand, the (0 0.5 8) (family B, off resonance) appears at \( T^* \), which coincides with the DC resistivity maximum, and shows an approximately linear dependence with temperature (see Fig. S5 for further reflections [33]). These differences imply that A and B are sensitive to different atomic displacements allowed in the CDW state and that the displacements that dominate B have a correlation to the transport properties. The previously reported difference in the onset temperatures (\( \approx 7 \) K) of (1.5 1.5 0.5) and (2.5 1 0) [20] as well as the linear temperature dependence of (2.5 1 0) are reasonably explained by a fourth-order contribution of the in-plane CDW distortion occurring at \( T_{\text{CDW}} \) [31]. However, the observed difference in the onset temperatures (\( \approx 37 \) K) in our study cannot be explained in the same way since a calculated fourth-order contribution to the intensity [black curve in Fig. 2(a)] does not fit the experimentally obtained data for (0 0.5 8).

The (0 0.5 9.5) reflection, which is space-group forbidden in the CDW state, is observed only around the Se K edge as seen in Fig. 3(a). The intensity depends on the azimuthal angle, and the profile is nicely described by \textit{ab initio} calculations performed by the FDMNES code using a model based on the crystal structure in the CDW state [32] [see Fig. 3(b)]. The polarization analysis at the specific azimuthal angle displayed in Fig. S3 is consistent with the calculated results where the reflection gives finite intensity in the \( \sigma - \pi' \) channel but no signal in the \( \sigma - \sigma' \) channel. On the basis of such profiles, which are well reproduced by our \textit{ab initio} calculations, and the symmetry analyses (see the Supplemental Material of [33]), the (0 0.5 9.5) space-group forbidden reflection intensity is explained by an aspheric electron distribution in the Se1 4p orbitals in the CDW state, also often called ATS (anisotropic tensor susceptibility) scattering [38].

The x-ray absorption at the Se K edge includes the excitation of an electron from the 1s state to the 4p valence state, which would be totally occupied in a fully ionic picture. Thus, the observation of the space-group forbidden reflection means that there are holes in the Se valence state in addition to the aspheric electron distribution in the Se1 4p, as predicted in Ref. [39] by DFT calculations. It is obvious that the change...
We find that $\delta$ function. not related to our observations since (2.5 1 0) is independent of the Supplemental Material [33] (see Ref. [33] for details of placements were carried out and are summarized in Table S2 A [3,4] generating holes in the Se $4p$ bands which influence the electron distribution of the Se.

To identify the nature of atomic displacements dominating space-group allowed reflections $A$ and $B$, numerical calculations for possible models with different types of displacements were carried out and are summarized in Table S2 of the Supplemental Material [33] (see Ref. [33] for details of the models and procedure). We find that $\delta_T$ and $\delta_{Se_{in}}$, both in-plane displacements, dominate $A$ while $\Delta_{Se_{e}}$, relating to an out-of-plane displacement, dominates $B$. Figure 4 shows the calculated intensities of the (0.5 1 1.5) and (0.5 0.5 8) reflections as function of $\delta_T$ and $\Delta_{Se_{e}}$ [the dependence on $\delta_{Se_{in}}$ shows a similar behavior to that of $\delta_T$, which is shown in Fig. S6(a) [33]]. $A$ is largely dominated by $\delta_T$ through a quadratic contribution to the intensity (linear in the structure factor) without any contribution from $\Delta_{Se_{e}}$. On the other hand, $B$ is dominated by $\Delta_{Se_{e}}$ ($\propto \Delta_{Se_{e}}^2$) with a 10$^3$ times smaller quartic contribution in $\delta_T$. The quartic contribution of $\delta_T$ to the intensity can explain the linear temperature dependence of $B$ but cannot explain the significant intensity and the difference in onset temperature from $A$. Thus, it is plausible that $\Delta_{Se_{e}}$ sets in $\approx$37 K lower than $T_{CDW}$ and develops slower as a function of temperature while cooling than the CDW order parameters reflected by $\delta_T$ and $\delta_{Se_{in}}$. These observations are possible when $\Delta_{Se_{e}}$ is not the primary order parameter of the CDW phase transition. The difference in onset temperatures between (1.5 1.5 0.5) and (2.5 1 0) reported earlier [20,31] are not related to our observations since (2.5 1 0) is independent of $\Delta_{Se_{e}}$ (as $I = 0$). As shown in Ref. [31], the temperature dependence of (2.5 1 0) is naturally explained by the quartic behavior of the in-plane displacements. However, the anomaly in the specific heat found in that study [20] might be directly related to $\Delta_{Se_{e}}$.

Whereas the CDW order largely affects the band structure, the maximum of the DC resistivity is not correlated to $T_{CDW}$ but $T^*$, around which the gyrotrropic electronic order also appears [5]. Note that $T_{CDW}$ can vary between different samples, probably due to differences in defect density [1]. The displacements $\delta_T$ and $\delta_{Se_{in}}$ dominate the CDW distortion and $\Delta_{Se_{e}}$ does not further break the symmetry in the CDW state. The $\Delta_{Se_{e}}$, the magnitude of which is much smaller than $\delta_T$ and $\delta_{Se_{in}}$, creates only a tiny change in the structure of the main bands that form the hybridization gap. The onset of $\delta_{Se_{in}}$ shortens the Se1-Ti bond length compared to Se2-Ti, and Se1 moves away from the adjacent Ti layer below $T^*$. This could weaken the orbital hybridization between Ti 3$d_{2z}$ and Se $4p_{x,z}$ at the A point, increasing the band curvatures of the specific branches [compare Figs. 1(c) and 1(d)]. Therefore, the carriers in Ti 3$d_{2z}$ and A-derived Se $4p_{x,z}$ would acquire lighter effective masses and longer mean free paths, resulting in a decrease of DC resistivity below $T^*$. Note that the Ti 3$d_{2z}$, which crosses the Fermi energy, dominates the transport in the CDW state. Carriers due to thermal fluctuations could additionally contribute to the transport [17].

Interestingly, for both Cu$_2$TiSe$_2$ ($x = 0.05$) and 1T'-TiSe$_2$ at $\geq$2.82 GPa, the anomalous peak in the DC resistivity vanishes and a superconducting state appears upon lowering the temperature [6,7]. These samples have the same space group and CDW transition as 1T'-TiSe$_2$ under ambient pressures, but the distortion $\Delta_{Se_{e}}$ is zero in the CDW state for both the doped and pressurized samples [32]. This implies that $\Delta_{Se_{e}}$ plays a critical role in the transport properties and might be a key parameter governing the emergence of the superconducting state.

We now comment on the possible occurrence of chirality in the CDW state. Even though the $B$ reflections have a lower onset temperature than $T_{CDW}$, a symmetry analysis based on the Landau theory valid for this second order phase transition is inconsistent with the occurrence of chirality [5]. The circular photogalvanic current, which is claimed as the evidence for a chiral electronic structure, appears at almost the same temperature as the structural modification [5]. This suggests that a possible chirality in the electronic states would be significantly coupled to the lattice, and therefore the underlying crystal lattice should be chiral. Observation of orbital asphericity through studying the polarization dependence of space-group forbidden reflections in resonant XRD is one of the established methods to determine the presence of chirality in crystal lattices and in orbital structures [40–42]. However, the observed polarization-dependent azimuthal-angle dependence of the (0.5 0.5 9.5) reflection is very well reproduced by the ab initio calculations assuming the nonchiral space group P3c1. Moreover, if the space group is P1 as claimed in earlier studies as a “chiral” space group [21–25], this reflection must be a symmetry allowed reflection. The absence of an intensity for this reflection at off resonance and in the $\sigma-\sigma'$ channel is shown in Figs. 3(a) and 3(b), respectively. This indicates that the reflection is space-group forbidden, ruling out possible chiral space groups, as well as the proposed space group P1.

FIG. 4. Numerically calculated intensities of (0.5 1 1.5) (green) and (0.5 0.5 8) (blue) reflections as functions of (a) $\delta_T$ and (b) $\Delta_{Se_{e}}$. The data are normalized by the intensity calculated for the reported structure in the CDW state [32]. The respective displacements are schematically displayed as insets. The green line in (a) and blue line in (b) represent a quadratic and the blue line in (a) a quartic function.
Therefore, we can conclude that our results give strong support for the absence of chirality of the Se orbitals (electronic and crystal structure) and speak against $P1$ symmetry (crystal structure) in the CDW state.

In summary, we examined the charge-density wave (CDW) phase of $1T$-TiSe$_2$ by means of x-ray diffraction. One of the studied three families of reflections has different onset temperature compared to the others. Our detailed analysis revealed that the family of reflections comes from the difference in relative out-of-plane motion between the two Se sites, which weakly couples to the CDW order. The consequent decrease of the effective mass of carriers results in a reduction of DC resistivity at lower temperatures. Our x-ray-diffraction results provide the crucial link between the origin of the anomalous feature in transport properties and structural modifications that change the hybridization in the relevant electronic bands. This specific picture clarifies now the microscopic origin of the transport properties of $1T$-TiSe$_2$. Experimental and model data are accessible from the Materials Cloud Archive [45].

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