T\textsubscript{d} to 1T\textsuperscript{'} structural phase transition in WTe\textsubscript{2} Weyl semimetal

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Elastic neutron scattering on a single crystal and powder X-ray diffraction measurements were carried out to investigate how the crystal structure evolves as a function of temperature in the Weyl semimetal WTe\textsubscript{2}. A sharp transition from the low-temperature orthorhombic phase (T\textsubscript{d}) to the high-temperature monoclinic phase (1T\textsuperscript{'}), was observed at ambient pressure in the single crystal near 565 K. Unlike in MoTe\textsubscript{2}, the solid-solid transition from T\textsubscript{d} to 1T\textsuperscript{'} occurs without the cell doubling of the intermediate T\textsubscript{d} phase with AABB (or ABBA) layer stacking. In powders however, the thermal transition from the T\textsubscript{d} to the 1T\textsuperscript{'} phase is broadened and a two phase coexistence was observed until 700 K, well above the structural transition.

I. INTRODUCTION

Transition metal dichalcogenides (TMDs) have attracted considerable attention recently because of their intriguing electronic band structure properties that render them hosts to exotic quasiparticles. MoTe\textsubscript{2} and WTe\textsubscript{2} are reported to be type-II Weyl semimetals in the orthorhombic T\textsubscript{d} phase\textsuperscript{[1,2]} due to spatial inversion symmetry breaking, and both show a large non-saturating magnetoresistance\textsuperscript{[3,4]}. They are layered structures, held together by van der Waals forces, and can undergo multiple solid-solid transitions through version symmetry breaking, and both show a large parameter \(\delta\)\textsuperscript{[3,4]}, as shown in Fig. 1(a). We define \(\delta\) as the distance along the \(a\)-axis between the midpoints of metal-metal bonds of neighboring layers; this definition is uniquely defined for both 1T\textsuperscript{'} (where it is related to the \(\beta\) angle) and T\textsubscript{d}.

With W substitution as in Mo\textsubscript{1−x}W\textsubscript{x}Te\textsubscript{2}, the 1T\textsuperscript{'} to T\textsubscript{d} structural transition temperature increases up until \(x \approx 0.57\)\textsuperscript{[4]}. However, it is not known at present whether this transition occurs at ambient pressure at the other end of the phase diagram with \(x = 1\) as in WTe\textsubscript{2}. A pressure-driven T\textsubscript{d}–1T\textsuperscript{'} structural transition has been reported to appear at 4 - 5 GPa\textsuperscript{[5]}, at 8 GPa\textsuperscript{[6]}, and in a broad range from 6.0 to 18.2 GPa, during which a volume collapse with dramatic changes in the lattice constants was observed\textsuperscript{[7]}. In MoTe\textsubscript{2}, pressure suppresses the temperature of the 1T\textsuperscript{'}–T\textsubscript{d} transition, and extinguishes it by \(\sim 1.2\) GPa\textsuperscript{[8,9]}, though dramatic changes in the lattice constants between the phases have not been reported. Nonetheless, the presence of a transition in WTe\textsubscript{2} under pressure, as well as the trend of increasing T\textsubscript{d}–1T\textsuperscript{'} transition temperature with W-substitution in the Mo\textsubscript{1−x}W\textsubscript{x}Te\textsubscript{2}\textsuperscript{[10,11]}\textsuperscript{[11] phase diagram suggest the possibility of an ambient-pressure transition at high temperatures.

Using elastic neutron scattering, we observed the T\textsubscript{d}–1T\textsuperscript{'} structural phase transition at ambient pressure in a single crystal of WTe\textsubscript{2}. The transition is sharp, occurs at \(\sim 565\) K, and proceeds without hysteresis. No intermediate phase is present across the phase boundary in WTe\textsubscript{2}, in contrast to the T\textsubscript{d} phase seen in MoTe\textsubscript{2}. From powder X-ray diffraction (XRD) however, the transition appears broad and incomplete up to 700 K, with phase coexistence across a wide temperature range.

II. EXPERIMENTAL DETAILS

The WTe\textsubscript{2} single crystals were grown out of a Te flux. First, WTe\textsubscript{2} powder was prepared from stoichiometric ratios of W and Te powders. The sintering was done in an evacuated quartz silica ampoule at 900 °C for 2 days. The sintered powder was then pressed into a pellet.
and sealed with excess Te in a molar ratio of 1:13. The ampoule was placed horizontally in a tube furnace and heated at a constant temperature of 850 °C for 7 days. Excess Te was removed by re-inserting one end of the ampoule into a tube furnace at ~900 °C and decanting the molten Te towards the cold end. For XRD, powder was sintered as described above.

Resistivity measurements under magnetic fields of 0 and 9 T are shown in Fig. 1(c). The residual resistivity ratio (RRR) from the 0 T data is calculated to be ~118(3). Our WTe2 crystals also have a large magnetoresistance, with a magnitude of 51,553% at 2 K under a 9 T magnetic field. These values are reasonably high [22], though higher values have been reported in the literature, such as an RRR of ~370 and a magnetoresistance of 452,700% at 4.5 K in an applied field of 14.7 T [1].

Elastic neutron scattering was performed on the triple axis spectrometer HB1A, located at the High Flux Isotope Reactor at Oak Ridge National Laboratory (ORNL). The elastic measurements used an incident neutron energy of 14.6 meV and the collimation was 40'-40'-S-40'-80'. The crystal was mounted on an aluminum plate via aluminum wire, and a furnace was used to control the temperature. Powder XRD measurements were collected as a function of temperature between 300 K and 700 K. Rietveld refinement was done using the GSAS-II software [23]. In this paper, we use atomic coordinates based on an orthorhombic unit cell (unless otherwise noted) with b < a < c (i.e., a ≈ 6.28 Å, b ≈ 3.496 Å, and c ≈ 14.07 Å).

III. RESULTS AND DISCUSSION

Shown in Figs. 1(d,e) are intensity maps which combine elastic neutron scattering scans along the (2, 0, L) at a sequence of temperatures on warming from 510 to 610 K, then cooling. A clear Td–1T' transition can be seen in the plots with the change in the Bragg peaks and without diffuse scattering. At low temperatures, the (202)Td and (203)Td Bragg peaks are observed. On warming, a structural phase transition into the 1T' phase is observed at ~565 K, followed by 1T' phase peaks appearing near L ≈ 2.2 and 2.8, similar to MoTe2. Unlike the appearance of the Td phase in MoTe2, there is no intermediate phase present in the transition in WTe2.

In Fig. 1(f), the intensities of the (203)Td and (203)1T, peaks, obtained from fits to scans along (2, 0, L), are plotted as a function of temperature on warming and cooling through the hysteresis loop. The transition from one phase to another is quite sharp with very little hysteresis. WTe2 shows a very different behavior from MoTe2 [11]. First, no hysteresis is observed between the Td→1T' transition on warming, and 1T'→Td transition on cooling. The warming and cooling data in Fig. 1(f) overlap. In contrast, in MoTe2, a hysteresis of tens of Kelvin is present in the Td–1T' transition, with a lingering hysteresis in the resistivity that can persist to hundreds of Kelvin [11]. Moreover, even the Td→Td′→Td loop which proceeds much more sharply than the transition between Td and 1T', has a hysteresis of ~5 K [11] in MoTe2. Second, the transition in WTe2 is narrower, with most of the transition occurring within a ~10K range. In MoTe2, the Td–1T' transition width is of the order of 30 K. The inter-

Figure 1. (a) The crystal structure of 1T'-Mo1-xWxTe2 projected in the a-c plane. (b) Stacking sequences for the Td and 1T' phases of WTe2. (c) Temperature and field dependence of resistivity in WTe2, for current along the b-direction and H || c. The relative error of each data point is ~0.001. (d,e) Scans of neutron scattering intensity along (2,0,L) collected on a single crystal of WTe2 on cooling and warming. The Bragg peak labelled D1 and D2 refer to the two 1T' twins. (f) Intensity as a function of temperature of ((203)Td and (203)1T), obtained from fits of scans along (2,0,L). (inset of (f)) The temperature dependence of the interlayer spacing, obtained from fits to longitudinal scans along (004).
layer spacing, determined from the position of the (004) Bragg peak in longitudinal scans and equivalent to \(c/2\) in the \(T_d\) phase, is plotted as a function of temperature in the inset of Fig. 1(f). No change in the interlayer spacing is seen across the transition (and the \(a\)-axis lattice constant must not change dramatically either, given the similar intensities of \((2, 0, L)\) scans which were performed across the transition without re-alignment), in contrast to the abrupt changes seen under pressure for the lattice constants [9].

Figure 2. The phase diagram of \(\text{Mo}_{1-x}\text{W}_x\text{Te}_2\) as a function of \(W\) concentration, \(x\), and temperature on cooling and warming. All data on this plot, except for \(\text{WTe}_2\), were first reported by us elsewhere [13]. The \(T_d\) and \(1T'\) phases are distinguished by the onset or completion temperatures at which 20% or 80% of the maximum intensity of the \((2, 0, 3)\) \(T_d\) peak is achieved. The vertical dashed lines represent different \(W\) fractions where neutron scattering measurements were taken.

Plotted in Fig. 2 is the phase diagram of \(\text{Mo}_{1-x}\text{W}_x\text{Te}_2\). The transition temperature increases continuously as a function of composition from \(\text{MoTe}_2\) to \(\text{WTe}_2\). The \(\text{Mo}_{1-x}\text{W}_x\text{Te}_2\) data up to \(x \sim 0.5\) were presented in Ref. [13]. There is a roughly linear increase in transition temperature with \(x\), though possibly increasing more slowly from \(x \sim 0.5\) to 1. The uncertainty in \(x\), which was determined indirectly from the layer spacing found via the position of the (004) Bragg peak in neutron scattering, is likely the source of the peak artifact near \(x \sim 0.5\). The narrowness of the \(\text{WTe}_2\) transition is striking relative to the broadness of the transition near \(x \sim 0.5\) [13]. Clearly, more research is needed from \(0.5 < x < 1\) to clarify how the narrow transition of \(\text{WTe}_2\) connects with the broader, hysteretic transition near \(x \sim 0.5\), even as both these transitions lack the complexity observed in the transition of \(\text{MoTe}_2\).

In contrast to the clean transition seen in the single crystal, evidence for a partial \(T_d\)–\(1T'\) transition is observed from powder XRD measurements of \(\text{WTe}_2\). From powder measurements from room temperature to 700 K, a two phase coexistence is observed, where the monoclinic phase grows out of the orthorhombic phase on warming.
The phase boundary from powder XRD is very broad, with the transition incomplete below ~700 K and accompanied by partial decomposition of the WTe$_2$ in contrast to the sharp transition observed in the single crystal (see Fig. 1). Shown in Figs. 3(a,b) are the Rietveld refinement results of the XRD data collected at 300 and 700 K on warming. WTe$_2$ is in the T$_d$ phase at 300 K and the data is fit using the orthorhombic symmetry. A secondary phase of WO$_2$ is present with a weight percent of ~5.4(2)%. Bragg peaks for a pure Te phase appear on further warming around ~600 K, steadily increasing with heating and reaching a weight percent of 9.90(22)% by 700 K. While the T$_d$ phase fits the data well at 300 K (Fig. 3(c-e)), by 700 K, the data are better fit by a combination of 1T$'$_WTe$_2$ and T$_d$-WTe$_2$ peaks (Fig. 3(f-h)). After first allowing the lattice constants of both phases to vary, the 1T$'$ lattice constants were fixed to be consistent with those found in the T$_d$ refinement, including having the monoclinic tilting angle $\beta$ be consistent with the values for the $\delta$ parameter derived from the T$_d$-refined atomic coordinates. With these assumptions, the 1T$'$ phase can be seen (in Fig. 3(f-h)) to contribute intensity to the sides of the T$_d$ peaks near 32.0°, 35.0°, and 43.5°. However, the intensity between the T$_d$ and T$_d$ peak positions suggests that disordered stacking, intermediate between T$_d$ and 1T$'$, is likely present. The fitted phase fractions are shown in Fig. 3(i). It can be seen that the transition is much broader in the single crystal, with the transition beginning between 500 and 600 K, and steadily increasing up to at least 700 K.

An essential parameter for the Mo$_{1-x}$W$_x$Te$_2$ structure is the $\delta$ parameter, which characterizes in-plane positioning of neighboring layers. From the refined coordinates of the T$_d$ phase XRD data, we obtained $\delta$ as a function of temperature (Fig. 3(j)). The $\delta$ parameter decreases by ~0.007 from 300 to 600 K, which is very similar to the decrease in Mo$_{0.91}$W$_{0.09}$Te$_2$ (~0.006 from 320 to 600 K.) For the 1T$'$ phase in the single crystal, we can obtain $\delta$ from the separation between opposite-twin 1T$'$ peaks, yielding 0.5482(3) at 610 K (and a monoclinic $\beta$ angle of 92.456(17)$^\circ$. This latter value is probably more reliable than those from powder refinement, which may be more insidiously affected by systematic errors due to the indirect nature of obtaining positions from Bragg peak intensities. Nevertheless, a rough agreement for $\delta$ is found between values found from the T$_d$-phase powder refinement and from the 1T$'$ peak splitting in the single crystal, as seen in Fig. 3(j)). The refined T$_d$-phase lattice parameters are shown in Fig. 3(k-m). Aside from a possible anomaly near 700 K, which may be related to the decomposition that results in the Te phase, or to the difficulty in getting uniquely fitted lattice constants in the presence of stacking disorder, we see the expected thermal expansion for a, b, and c.

Our finding of a T$_d$-1T$'$ structural phase transition in WTe$_2$ suggests that theories of the transition be revisited. The complexities of the transition in Mo$_{1-x}$W$_x$Te$_2$, such as the hysteresis, stacking disorder, and presence of the T$'_2$ phase have not been theoretically explained, but the relative stability of 1T$'$ over T$_d$ in MoTe$_2$ at higher temperature has been supported by the density functional theory calculations in Ref. [8]. Though that study’s calculations suggest that WTe$_2$ does not have a transition, in contrast to our findings, it does suggest a lack of an energy barrier along the transition path from 1T$'$ to T$_d$, which may be related to the lack of hysteresis seen in our single crystal data.

The structural trends shown in our data place constraints on theoretical models for the transition. We observed no detectable change in the interlayer spacing across the transition, similar to the negligible change seen in other Mo$_{1-x}$W$_x$Te$_2$ crystals [13]. (Kinks in interlayer spacing vs. temperature have been seen in some Mo$_{1-x}$W$_x$Te$_2$ crystals, but may be due to slight misalignment accompanying the transition [13].) This finding highlights the similarities between the phases, expected since they have nearly identical layers that are positioned relative to neighboring layers in nearly symmetry-equivalent ways. Such similarities may make sufficiently accurate calculations difficult, with subtle effects such as spin-orbit coupling contributing non-negligibly to the layer spacing [8]. Another structural factor to be considered is the dependence of the $\delta$ parameter on composition and temperature, though these trends are less constraining. Theory already appears to be consistent with the decrease in $\delta$ with W-substitution, with calculated values of $\delta = 0.540$ for WTe$_2$ vs. $\delta = 0.564$ for MoTe$_2$ (as extracted from calculated 1T$'$ lattice constants), and experimental values of 0.552 for our powder T$_d$-WTe$_2$ data vs. $\delta = 0.574$ reported for 1T$'$-MoTe$_2$ [18] (both at 300 K.) The similarity in the temperature-dependence of WTe$_2$ and Mo$_{0.91}$W$_{0.09}$Te$_2$ [13] suggests that these compositions have a similar anharmonicity in the interlayer potential, despite the difference in $\delta$.

There are several possible explanations for the broadness of the transition in WTe$_2$ powder as compared to single crystals. First, Te vacancies may be responsible, as they have been proposed to broaden the transition in MoTe$_2$ crystals [24]. We would expect that powder would have more decomposition than a single crystal due to a greater surface area to volume ratio. However, XRD refinement of the WTe$_2$ powder showed no evidence of Te vacancies; a refinement of 700 K data with the Te occupancy of all atoms in T$_d$- and 1T$'$-WTe$_2$ fixed to a single value yielded a composition of WTe$_{1.998(23)}$. A second possibility is that the transition is broadened in the small crystallites of a powder sample. In thin MoTe$_2$ crystals (hundreds of nm or less) the transition is known to be broadened or suppressed completely [25,27]. Third, there are likely more defects in powder, induced during sintering or grinding. Defects may frustrate layer sliding, and the presence of grain boundaries would frustrate the shape change expected in each grain’s orthorhombic-to-monoclinic transition. A better understanding of non-ideal behavior, such as that of powder, may help in realizing the potential of stacking changes to influence prop-
properties in quasi-two-dimensional materials.

IV. CONCLUSION

Using elastic neutron scattering on single crystals and XRD on powder samples of WTe$_2$, we observed a T$_d$-1T' structural phase transition in the Weyl semimetal WTe$_2$ at ambient pressure. In the crystal, the transition occurs at $\sim$565 K without hysteresis, but in the powder, the transition is broadened and incomplete up to 700 K. Our results place constraints on theories of the structural behavior of Mo$_{1-x}$W$_x$Te$_2$, which thus far have not predicted a transition in WTe$_2$.

Note added. During our investigations, we became aware of a submitted conference abstract reporting resistivity and X-ray diffraction data indicating a structural phase transition in WTe$_2$ at 613 K.

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