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Raman scattering studies

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Structural contributions to the pressure-tuned charge-density-wave to superconductor transition in ZrTe_3 : Raman scattering studies

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Superconductivity evolves as functions of pressure or doping from charge-ordered phases in a variety of strongly correlated systems, suggesting that there may be universal characteristics associated with the competition between superconductivity and charge order in these materials. We present an inelastic light (Raman) scattering study of the structural changes that precede the pressure-tuned charge-density-wave (CDW) to superconductor transition in one such system, ZrTe_3 . In certain phonon bands, we observe dramatic linewidth reductions that accompany CDW formation, indicating that these phonons couple strongly to the electronic degrees of freedom associated with the CDW. The same phonon bands, which represent internal vibrations of ZrTe_3 prismatic rods, are suppressed at pressures above ~ 10 kbar, indicating a loss of long-range order within the rods, specifically amongst intrarod Zr-Te bonds. These results suggest that the pressure-induced suppression of CDW order observed in ZrTe_3 is structurally driven, and provide insights into the origin of pressure-induced superconductivity in this material.

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I. INTRODUCTION

One of the most exciting areas of condensed matter research involves the study of how superconductivity evolves from magnetic- or charge-ordered phases in a diverse range of strongly correlated systems, including high T_c cuprates,¹ iron-arsenide superconductors,² and charge density wave materials.^{3–6} While the presence of secondary ordered phases are generally inimical to superconductivity in conventional superconductors, there is growing evidence that the optimal conditions for superconductivity in some unconventional superconductors may require some phase competition, and perhaps even phase coexistence.^{1,6}

A particularly interesting group of materials in which phase competition between charge and superconducting order appears to be important is charge-density-wave (CDW) materials that can be tuned to superconductor phases with either pressure or intercalation. Examples of these systems include intercalated⁴ and pressure-tuned³ 1T-TiSe_2 , intercalated TaS_2 ,⁷ pressure-tuned TbTe_3 ,⁸ intercalated HoTe_3 ,⁹ and intercalated^{10,11} and pressure-tuned¹² ZrTe_3 . These systems offer the opportunity to explore the competition between charge-order and superconductivity,^{3–6} and particularly the structural changes that enable the emergence of superconductivity as the CDW state collapses with increasing pressure or intercalation.

ZrTe_3 crystallizes in the ZrSe_3 -type structure (space group $P2_1/m$, shown in Fig. 1) in which ZrTe_3 trigonal prisms stack along the b axis to form infinite quasi-one-dimensional rods.¹³ The monoclinic unit cell contains two such rods, which are related by screw symmetry. Interprism Zr-Te bonds hold the rods together to form layers

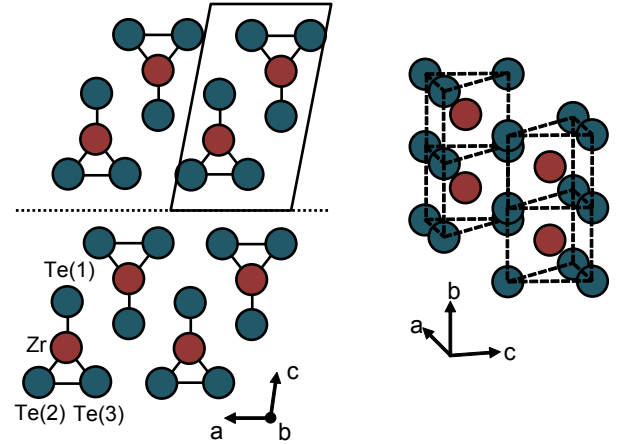


FIG. 1. (Color online) ZrTe_3 crystal structure. (left) Projection onto the ac plane. The dotted line represents the cleavage plane in this material. (right) Perspective showing two ZrTe_3 prismatic rods.

in the ab -plane which are easily cleaved along the c axis. Within each layer, Te(2) and Te(3) atoms form a dimerized chain along the a axis.¹³

Electronically, ZrTe_3 exhibits an anisotropic metallic resistivity below 300 K ($\rho_b \sim \rho_a \sim \rho_c/10$),^{11,14} and has resistive anomalies associated with CDW formation at $T_{CDW} = 63$ K¹⁴ and filamentary superconductivity below $T_c = 2$ K.¹⁵ The CDW transition in ZrTe_3 is associated with a commensurate structural modulation of wavevector $\mathbf{q} = (1/14, 0, 1/3)$,^{11,14,16} and most

strongly affects the conductivity perpendicular to the prismatic rods.¹⁴ A Kohn anomaly associated with a soft phonon mode¹⁷—as well as CDW fluctuations that extend well above T_{CDW} ^{18,19}—have been identified with the CDW transition in ZrTe_3 . Both band structure calculations^{13,20} and angle-resolved photoemission spectroscopy measurements¹⁸ indicate that the dimerized chains of $\text{Te}(2)$ - $\text{Te}(3)$ atoms along the a axis yield quasi-1D electronlike sheets of Fermi surface, and that nesting of these sheets may be responsible for CDW formation.

The application of hydrostatic pressure initially increases T_{CDW} with increasing pressure up to ~ 10 kbar (1 GPa), but increasing the pressure above ~ 20 kbar suppresses T_{CDW} , eventually leading to a complete suppression of CDW order above 50 kbar.¹² Increasing hydrostatic pressure also initially suppresses superconductivity for pressures greater than 5 kbar,¹² but reentrant superconductivity is observed for pressures above 50 kbar, i.e., above the pressure at which CDW behavior is suppressed.¹² Cu- and Ni-intercalation have also been shown to suppress the charge density wave state and induce superconductivity in ZrTe_3 .^{10,11}

While much is known about the complex phase diagrams of pressure-tuned and intercalated ZrTe_3 systems, several key issues concerning the underlying mechanisms governing the CDW-to-superconductor transitions remain uncertain. In particular, neither the relationship between the collapse of CDW order and the emergence of superconductivity in these systems, nor the nature of the structural changes that accompany this evolution, are well understood. These unresolved issues—which also confront a much broader range of materials exhibiting CDW-to-superconductor transitions^{3–7}—provide impetus for investigating the CDW-to-superconductor transition in ZrTe_3 using methods capable of probing the underlying structural changes associated with this transition.

We have used variable-temperature and variable-pressure inelastic light (Raman) scattering to investigate the microscopic details underlying the pressure-induced phases of ZrTe_3 . Phonon Raman scattering is particularly effective for studying the complex structural phases and changes in electron-phonon coupling that accompany temperature- and pressure-dependent phase changes in correlated materials such as ZrTe_3 , because this technique can convey detailed information about changes associated with specific atomic elements of the unit cells. In this paper, we show that certain phonon bands undergo dramatic linewidth reduction near T_{CDW} , indicating that these phonons couple strongly to the electronic degrees of freedom associated with the CDW. The same phonon bands, which represent internal vibrations of the ZrTe_3 prismatic rods, are suppressed at pressures above ~ 10 kbar. This indicates a pressure-induced loss of long-range order within the rods, specifically amongst intrarod Zr-Te bonds. We also find structural evidence for pressure-induced dimensional crossover in ZrTe_3 . These results suggest a structural mechanism for the observed

suppression of CDW formation above ~ 20 kbar and provide insights into the origin of pressure-induced superconductivity in ZrTe_3 .

II. EXPERIMENT

A. Sample preparation

Single crystals of ZrTe_3 were prepared at Brookhaven National Laboratory by chemical vapor transport, using a nearly stoichiometric mixture of powdered Zr and Te that was enclosed in an evacuated and sealed quartz ampoule along with iodine as the transport agent.^{10,11} The furnace gradient was kept between 760 and 650 C after heating to 700 C for two days. Crystals were oriented using a Panalytical X'pert single-crystal x-ray diffractometer with $\text{Cu K}\alpha_1$ radiation.

B. Raman scattering measurements

Raman scattering measurements were performed using the 647.1 nm excitation line of a Kr^+ laser. The incident laser power was limited to 5 mW and was focused to a ~ 50 μm -diameter spot to minimize laser heating of the samples; consequently, it was assumed that there was a negligible increase in the sample temperature from laser heating. The scattered light from the samples was collected in a backscattering geometry, dispersed through a triple-stage spectrometer, and then recorded with a liquid-nitrogen-cooled CCD detector. The incident light polarization was selected with a polarization rotator, and the scattered light polarization was analyzed with a linear polarizer, providing symmetry information about the excitations studied.

Variable-pressure and variable-temperature measurements were performed using a miniature cryogenic diamond anvil cell inserted into a helium-flow-through cryostat.²¹ This high pressure cell allows for *in situ* pressure adjustment, enabling Raman scattering measurements at temperatures 3–300 K and pressures 0–100 kbar. A liquid-argon medium was used to provide quasi-hydrostatic pressure. The pressure was determined from the shift in the R_1 fluorescence line of a ruby placed near the sample.²²

III. RESULTS AND DISCUSSION

A. Identification of phonon modes in ZrTe_3

Raman scattering has been used previously to measure the phonon spectrum of ZrTe_3 at room temperature²⁴ and at $T = 77$ K.²⁵ Fig. 2 shows our measurements of the phonon spectra of ZrTe_3 at $T = 295$ K and 6 K, obtained in a $(\mathbf{E}_i, \mathbf{E}_s) = (a, a)$ scattering geometry, where

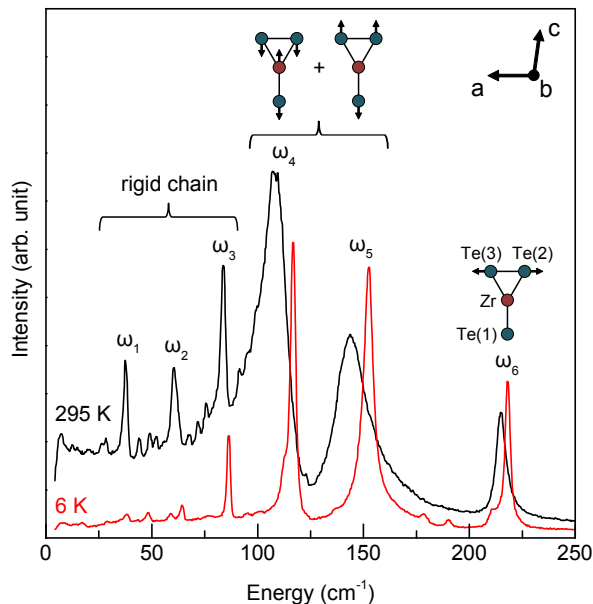


FIG. 2. (Color online) Raman spectra of ZrTe_3 at $T = 295$ K and $T = 6$ K with normal mode displacement patterns. Phonons $\omega_1 - \omega_3$ involve vibrations of rigid ZrTe_3 rods against one another. Phonons ω_4 and ω_5 involve deformations of the ZrTe_3 rods along the c axis. Phonon ω_6 is a diatomic vibration. Eigenmode illustrations after Ref. 23.

$\mathbf{E}_i$ and $\mathbf{E}_s$ are the incident and scattered light polarization directions, respectively. The $T = 295$ K phonon spectrum of ZrTe_3 exhibits six first-order phonon modes at $\omega_1 = 38 \text{ cm}^{-1}$, $\omega_2 = 60 \text{ cm}^{-1}$, $\omega_3 = 84 \text{ cm}^{-1}$, $\omega_4 = 108 \text{ cm}^{-1}$, $\omega_5 = 144 \text{ cm}^{-1}$ and $\omega_6 = 215 \text{ cm}^{-1}$. These energies are similar to those obtained previously.^{24,25}

As mentioned, the ZrTe_3 crystal may be viewed as infinite rods of ZrTe_3 trigonal prisms that are held together by interprism Zr-Te bonds. The phonon spectra of isostructural crystals ZrS_3 and ZrSe_3 are comprised of two sets of three vibrations that are well separated in energy²⁵, encouraging a normal mode description that discriminates between ‘external’ or prismatic-rod-preserving vibrations, and ‘internal’ or prismatic-rod-distorting vibrations. Although the two sets of vibrations are not as well separated in ZrTe_3 (see Fig. 2), we nevertheless follow previous authors^{23,24,26} in assigning lower-energy modes $\omega_1 - \omega_3$ to primarily external vibrations of the trigonal prismatic rods, and higher-energy modes $\omega_4 - \omega_6$ to primarily internal vibrations of the trigonal prismatic rods. These assignments are supported by the distinct pressure dependences of the external and internal mode frequencies (see section III C), as well as the symmetry considerations described below.

In the limit of weak interrod bonding, such that the $2mm$ symmetry of the rods predominates, the (a,a) scattering geometry used in this experiment allows for the observation of only 3 A_1 internal vibrations. One of these, a

‘diatomic’ vibration of the $\text{Te}(2)\text{-Te}(3)$ bond, is assigned to ω_6 following previous lattice dynamical calculations.²⁶ The other two internal vibrations, which involve deformations of the trigonal prisms along the c axis, are assigned to ω_4 and ω_5 . As interrod bonding becomes more significant, the $2/m$ crystal symmetry allows for the observation of up to five additional vibrations ($A_1 + 4 B_2$) in the (a,a) scattering geometry, including three external vibrations of the prismatic rods.²⁷ These rod preserving modes are assigned to the relatively weaker, lower energy modes $\omega_1 - \omega_3$.

In addition to the sharp phonon modes shown in Fig. 2, at $T = 295$ K there is a broad background that is likely associated with inelastic electronic scattering. This interpretation is supported by the broad linewidths of the ω_4 and ω_5 phonon modes, and especially by the asymmetric Fano lineshape²⁸ of the ω_4 phonon mode, suggesting that these modes are particularly strongly coupled to the underlying electronic background.

Several weak features appear in the $T = 6$ K spectrum, for example the peaks between $\omega = 175\text{--}200 \text{ cm}^{-1}$. These features likely represent phonons that have been folded to $k = 0$ from elsewhere in reciprocal space due to the CDW modulation of the structure. As can be seen in the following sections, these peaks vanish when the system is tuned out of the CDW phase via either temperature or pressure.

B. Temperature dependence of phonon modes in ZrTe_3

The temperature dependence of the Raman spectrum of ZrTe_3 is shown in Fig. 3(a), with the temperature dependences of the phonon band linewidths summarized in Fig. 3(b). The rigid rod phonon modes ω_2 and ω_3 , along with the diatomic mode ω_6 , show little linewidth dependence on decreasing temperature. On the other hand, vibrations ω_4 and ω_5 , which involve deformations of the ZrTe_3 trigonal prisms along the c axis, exhibit dramatic changes in linewidth as a function of decreasing temperature. In particular, between $T = 200$ K and 5 K the linewidths of the ω_4 and ω_5 bands decrease by factors of ~ 4.5 and ~ 3.5 , respectively (see Fig. 3(b)). The spectral range considered in this experiment did not include the lowest-energy external mode ω_1 .

The large reduction in linewidth of the ω_4 and ω_5 bands that accompanies CDW formation indicates a strong coupling between these vibrations and the electronic states associated with the CDW. As mentioned, CDW modulation in ZrTe_3 opens a gap 2Δ in the dispersion of the electronic band arising from the $5p$ orbitals of $\text{Te}(2)$ and $\text{Te}(3)$ ions^{13,29}. The size of 2Δ was found^{19,29} to be at least 400 cm^{-1} , i.e., larger in energy than the vibrations considered here. Therefore, the reduction in linewidth of modes ω_4 and ω_5 as the gap is opened reflects a loss of electronic relaxational channels for these particular vibrations. Such linewidth changes have also been ob-

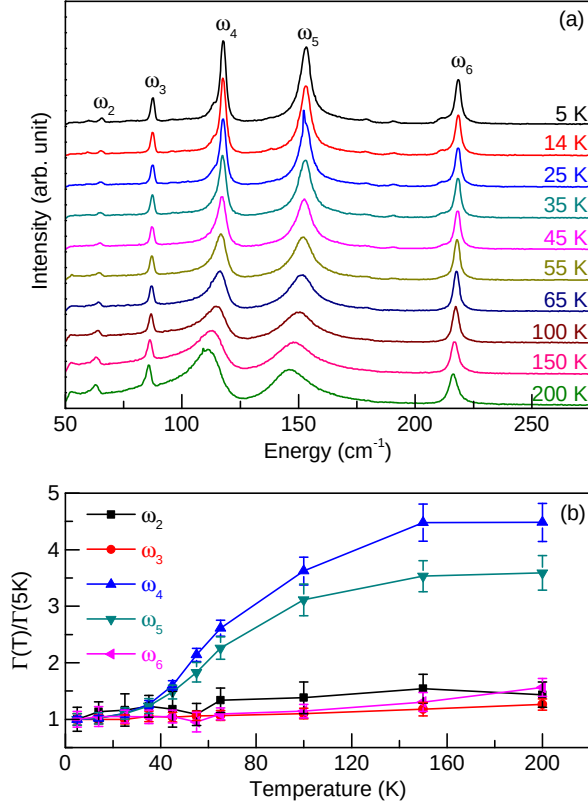


FIG. 3. (Color online) (a) Temperature dependence of the ZrTe₃ Raman spectrum at ambient pressure. Spectra have been offset for clarity. (b) Phonon band linewidths, relative to $T = 5$ K, as a function of temperature.

served for strongly coupled phonons in other correlation gap materials, such as the putative Kondo insulator FeSi and the A-15 superconductor Nb₃Sn.^{30,31} On the other hand, the lower-energy external vibrations are evidently not strongly coupled to the relevant electronic degrees of freedom, as their linewidths are insensitive to the formation of the CDW (see Fig. 3(b)). Remarkably, the linewidth of the diatomic vibration ω_6 is also largely insensitive to the electronic gap formation, despite the fact that this mode represents a longitudinal vibration of the dimerized Te(2)-Te(3) chain.

C. Pressure dependence of phonon modes in ZrTe₃

The pressure dependence of the Raman spectrum of ZrTe₃ is shown for $T = 3$ K in Fig. 4(a), with the pressure dependences of the ω_2 – ω_6 mode frequencies summarized in Fig. 4(b). The frequencies of internal modes ω_4 – ω_6 show relatively little sensitivity to applied pressure, while the frequencies of external modes ω_2 and ω_3 , which stretch the interrod Zr-Te bonds, increase linearly as a function of pressure. This indicates that interrod coupling becomes stronger at high pressures, or equivalently,

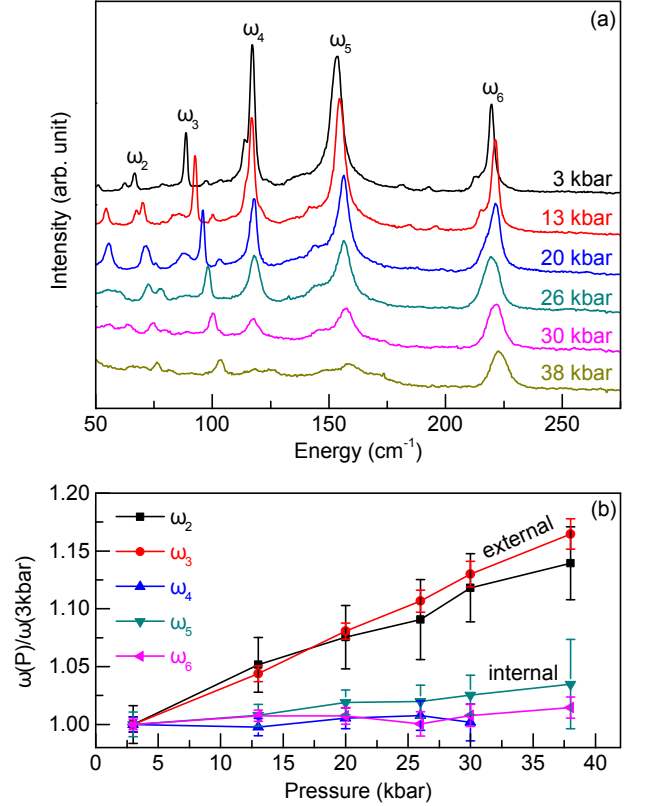


FIG. 4. (Color online) (a) Pressure dependence of the ZrTe₃ Raman spectrum at $T = 3$ K. Spectra have been offset for clarity. (b) Phonon energies, relative to $P = 3$ kbar, as a function of pressure.

that the crystal becomes more three-dimensional. Increased three-dimensionality and the resultant reduction in nested Fermi surface has been speculated to contribute to the pressure-induced suppression of the CDW above ~ 20 kbar in ZrTe₃.¹² Similar pressure-induced transitions between CDW and superconducting phases caused by enhanced interrod coupling have also been observed in the quasi-1D rod materials NbSe₃ and Nb₃Te₄.^{32,33} The decreased one-dimensionality of ZrTe₃ with pressure also suggests that pressure-induced superconductivity in ZrTe₃ will not have the filamentary nature that characterizes the ambient pressure superconductivity.^{15,34}

The most striking feature of the spectra shown in Fig. 4(a) is the suppression of internal vibration peaks ω_4 and ω_5 with applied pressure. Whereas warming through the CDW transition broadens peaks ω_4 and ω_5 by a factor of 3.5–4.5 due to an increase in carriers, increasing pressure has a much smaller ($< 50\%$) effect on the linewidths of these peaks. The pressure-induced loss of integrated intensity of peaks ω_4 and ω_5 is therefore most likely due to a loss of long-range structural order, rather than overdamping due to electron-phonon coupling. To be more specific, we note that the suppressed modes ω_4 and ω_5 primarily stretch intraprisim Zr-Te bonds. On the other

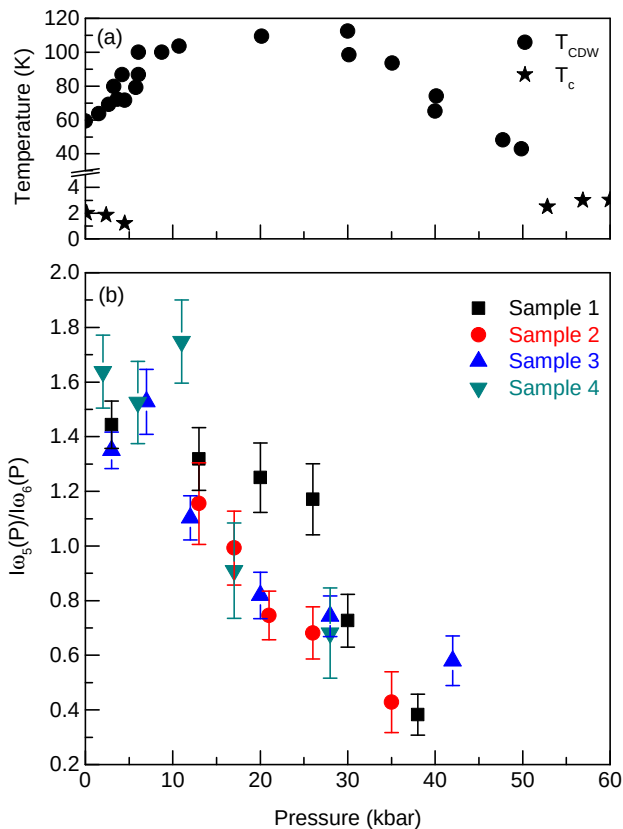


FIG. 5. (Color online) (a) Pressure dependence of the CDW transition temperature T_{CDW} and the superconducting transition temperature T_c , from Ref. 12. (b) Pressure dependence of the peak intensity of intra-prismatic-rod mode ω_5 relative to mode ω_6 . Data shown are from measurements of four different samples.

hand, the lower-energy external vibrations ω_2 and ω_3 , which primarily involve interprism Zr-Te bonds, as well as the diatomic vibration ω_6 of the Te(2)-Te(3) bond, all persist up to the highest pressures measured. Therefore, the pressure-induced loss of long-range order and suppression of modes ω_4 and ω_5 is likely due to disorder amongst the intraprism Zr-Te bonds.

Figure 5(b) shows the pressure-dependence of the peak intensity of the ω_5 band, relative to the robust ω_6 band. For comparison, Fig. 5(a) shows the evolution of T_{CDW} (filled circles) as a function of pressure. The peak intensity decreases rapidly above ~ 10 kbar, and is almost completely suppressed at pressures approaching the CDW collapse at ~ 50 kbar. Since the ω_4 and ω_5 vibrations have already been shown to be strongly coupled to the electronic degrees of freedom involved in CDW formation, and since the suppression of T_{CDW} follows the suppression of modes ω_4 and ω_5 , it is natural to associate the disorder amongst intraprism Zr-Te bonds with the collapse of the CDW. In support of this interpretation, we note that a recent *ambient*-pressure study of single-crystal ZrTe₃ grown at elevated temperatures also observed sup-

pression of the CDW in favor of superconductivity.³⁵ This was attributed to random displacements of the Zr and Te(1) atoms along the c axis as measured with x-ray diffraction, which is an interpretation quite similar to the pressure-induced structural changes proposed in our study. High-pressure x-ray-diffraction measurements of pure ZrTe₃ would be useful for confirming this interpretation of our high-pressure results.

The pressure dependences of the ZrTe₃ optical phonons demonstrate not only a trend toward higher-dimensionality, which may explain the pressure-induced suppression of the CDW in general terms via a loss of nested Fermi surface, but also indicate a specific structural change that appears to precede CDW collapse; namely, a loss of long-range order in the ZrTe₃ trigonal prismatic rods.

IV. SUMMARY

We have performed variable-temperature Raman measurements of ZrTe₃ which show that certain ZrTe₃-rod-deforming vibrations exhibit dramatic linewidth reductions that accompany CDW formation in this crystal, indicating that these vibrations are strongly coupled to the electronic states involved in the formation of the CDW. We have also performed variable-pressure Raman measurements which show that the same ZrTe₃-rod-deforming vibrations are strongly suppressed at pressures above ~ 10 kbar, mirroring the previously-observed pressure-induced suppression of the CDW. We argue that this suppression reflects a loss of long-range structural order at high pressures, specifically amongst the intrarod Zr-Te bonds, and that such a structural degradation may be responsible for the eventual pressure-induced collapse of the CDW.

Note added in proof. As this manuscript was in submission, we became aware of a variable-temperature Raman investigation of the ZrTe₃ vibrational modes by Hu et al. which shows good agreement with our variable-temperature experimental results.³⁶ Their calculation of the normal mode displacement patterns indicates that modes ω_4 and ω_5 have some longitudinal character along the a axis, i.e., stretch the Te(2)-Te(3) bonds. This may explain the strong coupling between these vibrations and the gapped electronic states, as the polarization of the soft phonon in ZrTe₃ has a large component along this direction.¹⁷ It may also mean that the structural degradation that instigates the suppression of CDW order involves the Te(2)-Te(3) bonds in addition to the intrarod Zr-Te bonds. Our essential conclusion—that the pressure-tuned CDW-to-superconductor transition in ZrTe₃ appears to be structurally driven—remains unchanged.

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