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## Pressure effect on the Curie temperature and thermal expansion of CrTe

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**Abstract.** The pressure  $P$  derivative  $dT_C/dP$  of the Curie temperature  $T_C$ , the linear magnetostriction  $\Delta l/l$  at 4.2 K, the lattice parameters  $a$  and  $c$  as functions of temperature  $T$  and the high-temperature paramagnetic susceptibility  $\chi$  of CrTe have been measured. The value of  $dT_C/dP$  is found to be  $-7.0 \pm 0.2$  K kbar<sup>-1</sup>. Thermal expansion anomalies of both  $a$  and  $c$  below  $T_C = 350 \pm 2$  K are observed upon cooling. The inverse of  $\chi$  above  $T_C$  shows a break at about 600 K. The field derivative  $d(\Delta l/l)/dH$  in the interval  $40 \text{ kOe} < H < 78 \text{ kOe}$  at 4.2 K is found to be  $1.2 \times 10^{-9}$  Oe<sup>-1</sup>. The results obtained are discussed on the basis of an appropriate thermodynamic relation, together with the reported results on  $dT_C/dP$  and the thermal expansions of Cr<sub>1- $\delta$</sub> Te.

### 1. Introduction

Chromium telluride CrTe with the NiAs-type crystal structure is a ferromagnet with a Curie temperature  $T_C = 331\text{--}347$  K [1], as shown in table 1. The value of  $T_C$  for Cr<sub>1- $\delta$</sub> Te remains nearly constant in the small- $\delta$  region while it steeply decreases with increasing  $\delta$  beyond  $\delta = 0.25$  (figure 1(a)). Of the 3d transition-metal monochalcogenides, CrTe is the only ferromagnet. The pressure effect on  $T_C$  of CrTe has been intensively studied because of interest in the distance dependence of the exchange interactions between the magnetic atoms and the stability of ferromagnetism in the Cr<sub>1- $\delta$</sub> Te system. However, the values of the pressure derivative  $dT_C/dP$  of  $T_C$  in Cr<sub>1- $\delta$</sub> Te are scattered over a wide range from  $-5.5$  to  $-6.8$  K kbar<sup>-1</sup> (table 1). The negative  $dT_C/dP$  remains nearly constant in the interval  $0 \leq \delta \leq 0.25$ , while it rapidly increases with increasing  $\delta$  from about  $-6$  to  $-2$  K kbar<sup>-1</sup> in the interval  $0.25 < \delta \leq 0.35$  (figure 1(b)). It is of interest to investigate the  $\delta$ -dependence of  $dT_C/dP$  for CrTe in order to consider the relation between the pressure effect on  $T_C$  and the magnetic properties of Cr<sub>1- $\delta$</sub> Te during the course of our investigation of the magnetic properties of the 3d- and 4d-metal-substituted Cr<sub>1- $\delta$</sub> Te system. In the present paper, we report the effect of the hydrostatic pressure  $P$  on  $T_C$ , the thermal expansion in the temperature  $T$  range between 15 and 800 K, the magnetic susceptibility  $\chi$  at temperatures above  $T_C$  and the linear magnetostriction  $\Delta l/l$  at 4.2 K in a magnetic field  $H$  of up to 76 kOe.

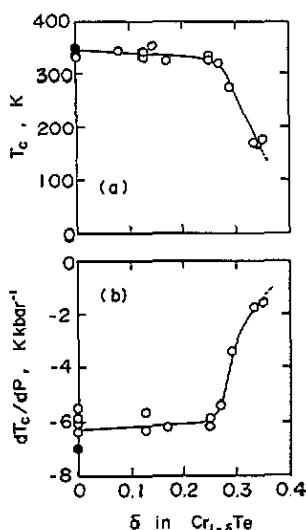


Figure 1. (a) Curie temperature  $T_C$  and (b) pressure derivative  $dT_C/dP$  of  $T_C$  as functions of  $\delta$  for  $\text{Cr}_{1-\delta}\text{Te}$ :  $\bullet$ , present data;  $\circ$ , data mainly taken from [1, 8].

Table 1. Curie temperature  $T_C$  and the pressure derivative  $dT_C/dP$  of  $T_C$  for  $\text{CrTe}$ .

$T_C$ (K)	$dT_C/dP$ (K kbar $^{-1}$ )	Reference
331	$-5.9 \pm 0.3$	[2]
338	$-6.1$ (0 kbar < $P$ < 2.45 kbar)	[3]
	$-6.8$ (2.45 kbar < $P$ < 3.92 kbar)	
335	$-5.5$	[4]
343	$-5.5$	[5]
347	$-6$	[6]
342	$-6.2 \pm 0.2$	[7]
350	$-7.0 \pm 0.2$	This work

## 2. Experimental procedure

A 1:1 mixture of Cr (99.99% pure) and Te (99.99% pure) grains was sealed in an evacuated silica tube. The mixture was heated to 800°C for 3 d. The product was ground and pressed at 1 t cm $^{-2}$  into discs. They were sintered at 1000°C for 2 d and subsequently at 800°C for 10 d. Finally, they were quenched into water. The powder x-ray diffraction pattern obtained for the sample can be explained in terms of the NiAs-type crystal structure and no foreign peak was detected. The lattice parameters  $a$  and  $c$  at room temperature, the cell volume  $V$  and the axial ratio  $c/a$  are determined to be 4.0108 Å and 6.2526 Å, 87.104 Å $^3$  and 1.559, respectively. The measurement of  $\chi$  as a function of  $T$  was carried out using a Faraday-type magnetic balance. The linear magnetostriction was measured using the usual strain gauge method. The measurement of the temperature dependences of  $a$  and  $c$  is carried out in heating runs using the same method [9] as reported previously. The initial permeability  $\mu$  at various pressures was measured using a piston-cylinder-type apparatus in heating runs.

## 3. Results

Figure 2 shows the typical temperature dependence of  $\mu$  at various pressures. As seen in the figure,  $\mu$  at ambient pressure strongly decreases around 350 K with increasing temperature.

Here,  $T_C$  was assigned as the intersection point of the two full lines, as shown in figure 2. At ambient pressure,  $T_C$  is determined to be  $350 \pm 2$  K. A similar temperature dependence of  $\mu$  to that at ambient pressure is also observed at higher pressures. The pressure dependence of  $T_C$  is shown in figure 3. As the pressure increases to 13.4 kbar,  $T_C$  linearly decreases with increasing pressure and the value of  $dT_C/dP$  is found to be  $-7.0 \pm 0.2$  K kbar $^{-1}$ . The values of  $T_C$  and  $dT_C/dP$  obtained in the present study are consistent with those for the previous studies, as summarized in table 1. Both values are among the largest obtained in the previous studies.

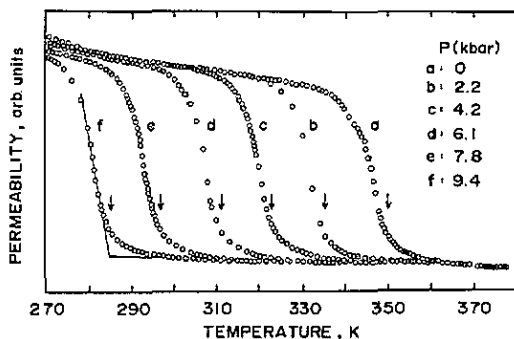


Figure 2. Typical temperature dependence of permeability around  $T_C$  for CrTe at various pressures. The downward arrows indicate  $T_C$ .

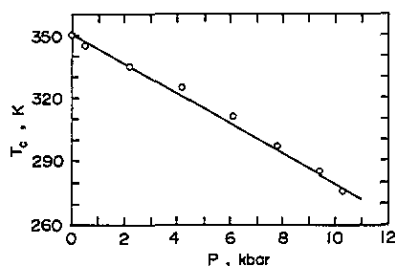


Figure 3. Pressure dependence of the Curie temperature  $T_C$  for CrTe.

Figure 4 shows the temperature dependences of  $a$  and  $c$  for CrTe in the temperature range between 15 and 800 K. As the temperature increases,  $a$  gradually decreases up to about 150 K and then subsequently increases on heating to 200 K. A first contraction is observed around 350 K, above which  $a$  increases linearly up to about 550 K. In contrast with the low-temperature behaviour of  $a$ ,  $c$  increases smoothly as the temperature increases to about 250 K. Also, a strong contraction is observed at about 350 K, above which  $c$  increases linearly up to about 550 K. The temperature where the strong contraction is observed around 350 K corresponds well to  $T_C$  which is determined in the  $\mu$  versus  $T$  curve at ambient pressure. From the temperature dependences of  $a$  and  $c$ , we can estimate  $\alpha_L$  ( $L = a, c$ ), the coefficient of linear thermal expansions below and above  $T_C$ . The values of  $\alpha_a(T < T_C)$  and  $\alpha_a(T > T_C)$  are determined to be  $-2.2 \times 10^{-5}$  K $^{-1}$  and  $0.3 \times 10^{-5}$  K $^{-1}$ , respectively,

and those of  $\alpha_c(T < T_C)$  and  $\alpha_c(T > T_C)$  to be  $-4.8 \times 10^{-5} \text{ K}^{-1}$  and  $0.8 \times 10^{-5} \text{ K}^{-1}$ , respectively. From these values, the differences between  $\alpha_L$  ( $L = a, c$ ) below and above  $T_C$  given by

$$\Delta\alpha_L = \alpha_L(T < T_C) - \alpha_L(T > T_C)$$

are found to be  $\Delta\alpha_a = -2.5 \times 10^{-5} \text{ K}^{-1}$  and  $\Delta\alpha_c = -5.6 \times 10^{-5} \text{ K}^{-1}$ . In the temperature range above about 550 K, a second contraction is observed in both  $a$  and  $c$  with increasing temperature. The fractional change in both  $a$  and  $c$  below and above 600 K are approximately 2% and 8%, respectively. Between 680 and 800 K, both  $a$  and  $c$  increase linearly with  $\alpha_a$  ( $680 \text{ K} < T < 800 \text{ K}$ ) =  $1 \times 10^{-5} \text{ K}^{-1}$  and  $\alpha_c$  ( $680 \text{ K} < T < 800 \text{ K}$ ) =  $2 \times 10^{-5} \text{ K}^{-1}$ , respectively.

Here, we consider the difference  $\Delta L$  ( $L = a, c$ ) between  $L_{\text{ferro}}(2T_C/3)$  at  $T = 2T_C/3$  in the ferromagnetic state and  $L_{\text{para}}(2T_C/3)$  in the paramagnetic state, as defined below:

$$\Delta L = L_{\text{ferro}}(2T_C/3) - L_{\text{para}}(2T_C/3).$$

The value of  $L_{\text{para}}(2T_C/3)$  is estimated from the straight extrapolation line from the paramagnetic state, as shown in the inset of figure 4. Figure 5 shows  $\Delta a$  and  $\Delta c$  as functions of  $\delta$  in  $\text{Cr}_{1-\delta}\text{Te}$ . The values of  $\Delta L$  ( $L = a, c$ ), which are taken from the data of the thermal expansions reported previously for  $\text{Cr}_{1-\delta}\text{Te}$  with  $0.014 \leq \delta \leq 0.33$  [10],  $\delta = 0.33$  [11] and  $\delta = 0.35$  [8], are plotted in this figure. As seen in the figure,  $\Delta a$  is nearly independent of  $\delta$ , while  $\Delta c$  decreases with increasing  $\delta$  and extrapolates to zero at about  $\delta = 0.33$ .

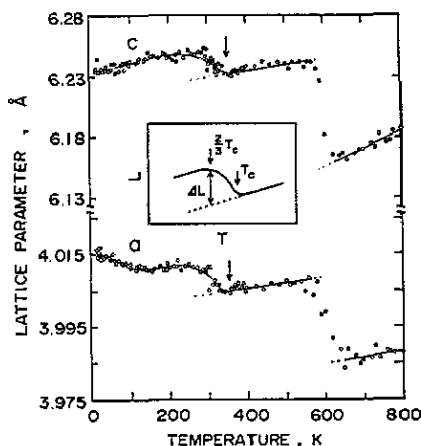


Figure 4. Lattice parameters  $a$  and  $c$  as functions of temperature for CrTe. The downward arrow indicates  $T_C$ . The inset shows the schematic definition of  $\Delta L$  ( $L = a, c$ ) at  $2T_C/3$ .

Figure 6 shows the temperature dependence of cell volume in the temperature range  $15 \text{ K} < T < 800 \text{ K}$ . A similar temperature dependence of  $V$  to that of  $a$  is also observed around  $T_C$  and above 600 K. The coefficients  $\beta$  of volumetric thermal expansion below and above  $T_C$  are determined to be  $\beta(T < T_C) = -8.1 \times 10^{-5} \text{ K}^{-1}$  and  $\beta(T > T_C) = 1.2 \times 10^{-5} \text{ K}^{-1}$ , respectively. From these values, the difference between  $\beta$  below and above  $T_C$  given by

$$\Delta\beta = \beta(T < T_C) - \beta(T > T_C)$$

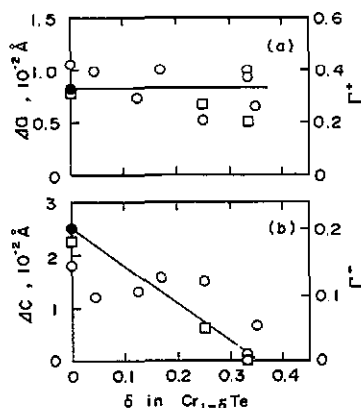


Figure 5. (a)  $\Delta a$  and  $\Gamma^+$  and (b)  $\Delta c$  and  $\Gamma^-$  as functions of  $\delta$  for  $\text{Cr}_{1-\delta}\text{Te}$ :  $\circ$ ,  $\Delta L$  ( $L = a, c$ ) from [8, 10, 11];  $\square$ ,  $\Gamma^s$  ( $s = +, -$ ) from [8, 10, 11];  $\bullet$ , present data.

is found to be  $-9.3 \times 10^{-5} \text{ K}^{-1}$ .

As shown in the inset of figure 6, the reciprocal of  $\chi$  ( $\text{emu mol}^{-1}$ ) above  $T_C$  increases smoothly up to about 600 K, above which it increases more rapidly. Tentatively, we analyse the  $\chi^{-1}$  versus  $T$  curve, assuming the Curie-Weiss law  $\chi = C_M/(T - \theta)$ . Here,  $C_M$  ( $\text{K emu mol}^{-1}$ ) is the molar Curie constant and  $\theta$  (K) the Weiss constant. The values of  $C_M$  and  $\theta$  are determined to be  $2.06 \text{ K emu mol}^{-1}$  and  $358 \text{ K}$ , respectively, in the interval  $360 \text{ K} < T < 600 \text{ K}$ , and  $1.11 \text{ K emu mol}^{-1}$  and  $460 \text{ K}$ , respectively, in the interval  $600 \text{ K} < T < 760 \text{ K}$ . From the values obtained for  $C_M$ , the effective number  $P_{\text{eff}}$  of Bohr magnetons per Cr atom for the two different temperature ranges is found to be  $4.1\mu_B$  in the interval  $360 \text{ K} < T < 600 \text{ K}$  and  $3.0\mu_B$  in the interval  $600 \text{ K} < T < 760 \text{ K}$ . Both values of  $P_{\text{eff}}$  are smaller than that ( $P_{\text{eff}} = 4.9\mu_B$ ) obtained when the  $\text{Cr}^{2+}$  state is assumed in CrTe. From the values of  $P_{\text{eff}}$ , the effective numbers  $q_c$  of Bohr magnetons per localized moment, derived from the high-temperature susceptibility, are found to be 3.22 and 2.36, respectively. The Rhodes-Wohlfarth ratio  $q_c/q_s$  is 1.3 in the interval  $380 \text{ K} < T < 600 \text{ K}$  and 0.9 in the interval  $600 \text{ K} < T < 800 \text{ K}$ . Here, the value of  $q_s = 2.45$  is used, as derived below.

Figure 7 shows the field dependence of  $\Delta l/l$ . As seen in the figure,  $\Delta l/l$  gradually increases with increasing  $H$  in the small- $H$  region and exhibits a linear increase above about 40 kOe up to 78 kOe. From the linear part of  $\Delta l/l$ , the field derivative  $d(\Delta l/l)/dH$  is found to be  $1.2 \times 10^{-9} \text{ Oe}^{-1}$  in the interval  $40 \text{ kOe} < H < 78 \text{ kOe}$ . We can estimate  $d\sigma_s/dP$ , the pressure derivative of spontaneous magnetization  $\sigma_s$ , from the thermodynamic relation

$$(d\omega/dH)_P = \rho(d\sigma_s/dP)_H$$

with  $\omega = 3(\Delta l/l)$ , where  $\omega$  is the volume strain and  $\rho$  the density of the sample. The estimated value of  $(d\sigma_s/dP)_H$  is  $-0.52 \text{ emu}^{-1} \text{ kbar}^{-1}$ . Here, the value of  $\rho$  used is  $6.85 \text{ g cm}^{-3}$ . The saturation magnetization  $\sigma_0$  at 20 K is reported to be  $76.2 \text{ emu g}^{-1}$  [12], which corresponds to the effective number  $q_s$  of Bohr magnetons, 2.45. Using this value of  $\sigma_0$ ,  $\sigma_s^{-1}(d\sigma_s/dP)_H$  is estimated to be  $-6.8 \times 10^{-6} \text{ bar}^{-1}$ .

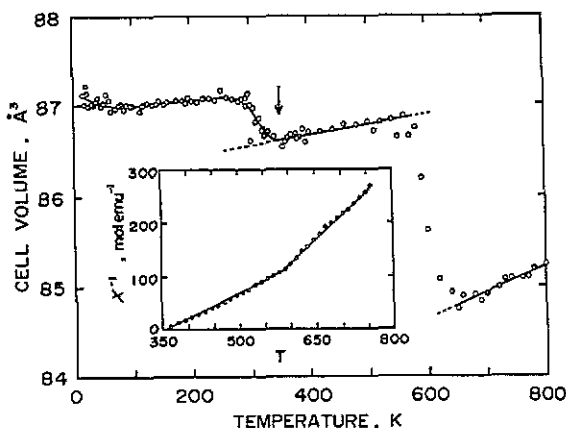


Figure 6. Cell volume as a function of temperature for CrTe. The downward arrow indicates  $T_C$ . The inset shows the reciprocal  $\chi^{-1}$  of the magnetic susceptibility for CrTe above  $T_C$ : —, curve drawn using the Curie constant  $C_M$  (emu K mol $^{-1}$ ) and the Weiss constant  $\theta$  (K), assuming the Curie-Weiss law  $\chi = C_M/(T - \theta)$  (see text).

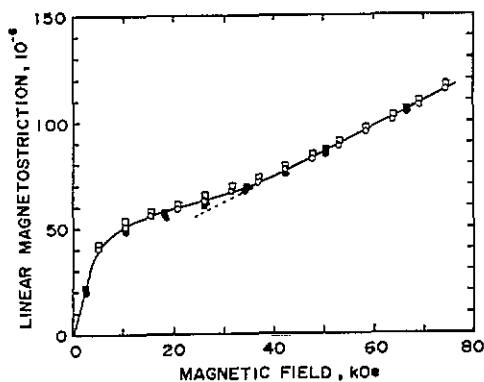


Figure 7. Linear magnetostriction  $\Delta l/l$  as a function of magnetic field for CrTe at 4.2 K: ○,  $\Delta l/l$  for increasing field in the first run; ●,  $\Delta l/l$  for decreasing field in the first run; □,  $\Delta l/l$  for increasing field in the second run; ■,  $\Delta l/l$  for decreasing field in the second run.

#### 4. Discussion

The negative value of  $(d\sigma_s/dP)_H$  at 4.2 K obtained in the present study suggests that the magnetic moment of the Cr atom is dependent on the volume even at absolute zero temperature. This cannot be explained by assuming the existence of the localized magnetic moment of the Cr atom. Furthermore, the value of  $(d\sigma_s/dP)_H$  is comparable with those for the Invar alloys [13]. The value of  $q_c/q_s$  in the interval  $360 \text{ K} < T < 600 \text{ K}$  is larger than unity. These indicate that CrTe can be classified as an itinerant ferromagnet. Therefore, the present results for  $dT_C/dP$ , the thermal expansion and  $\sigma_s$  should be considered on the basis of an itinerant ferromagnet. In the present discussion, the pressure derivative of  $T_C$  and the thermal expansions obtained for CrTe, together with those reported previously in the  $\text{Cr}_{1-x}\text{Te}$  system, are discussed qualitatively in terms of an appropriate thermodynamic

relation.

The pressure derivative of  $T_C$  in the second-order phase transition is given by the Ehrenfest relation

$$dT_C/dP = T_C V_{\text{mol}} \Delta\beta / \Delta C_p \quad (1)$$

where  $\Delta\beta$  and  $\Delta C_p$ , respectively, are the difference between the volumetric expansion coefficients and the difference between the heat capacities at  $T_C$ , and  $V_{\text{mol}}$  is the molar cell volume. The value of  $\Delta C_p$  for CrTe is obtained to be  $0.10 \text{ J g}^{-1} \text{ K}^{-1}$  [14]. Insertion of the values of  $\Delta\beta = -9.3 \times 10^{-5} \text{ K}^{-1}$ ,  $\Delta C_p = 18.03 \text{ J mol}^{-1} \text{ K}^{-1}$ ,  $V_{\text{mol}}(T = T_C) = 52.13 \text{ cm}^3 \text{ mol}^{-1}$  and  $T_C = 350 \text{ K}$  into (1) gives  $dT_C/dP = -9.4 \text{ K kbar}^{-1}$ , which is consistent with the present result. The thermal expansion anomalies in both  $a$  and  $c$  below  $T_C$  are in good agreement with those [7, 15, 16] reported previously. Similar behaviours have been observed for  $\text{Cr}_{1-\delta}\text{Te}$  with  $0.042 \leq \delta \leq 0.25$  [10] and  $0.35$  [8] except for  $\delta = 0.33$  ( $\text{Cr}_2\text{Te}_3$ ) [10, 11]. For  $\delta = 0.33$  ( $\text{Cr}_2\text{Te}_3$ ),  $c$  smoothly varies upon cooling through  $T_C$  and no thermal expansion anomaly is observed [10, 11]. The magnitude of thermal expansion is sensitive to the sample in terms of the condition for preparation and the transition region around  $T_C$  is very narrow. Therefore, the exact values of  $\Delta\alpha_L$  below and above  $T_C$  for the different  $\delta$  are difficult to estimate using the data reported previously. In the present paper, we consider the magnitude of  $\Delta L$  ( $L = a, c$ ), instead of  $\Delta\alpha_L$  ( $L = a, c$ ) for the different  $\delta$  in consideration of the relation between the pressure derivative of  $T_C$  and the thermal expansion anomalies.

In order to investigate qualitatively the relation between the  $\delta$  dependence of  $dT_C/dP$  and the thermal expansions along the  $a$  and  $c$  axes in  $\text{Cr}_{1-\delta}\text{Te}$ , we consider  $dT_C/dP$  under hydrostatic pressure associated with the strain derivative  $dT_C/de_L$  ( $L = a, c$ ) of  $T_C$ , where  $e_a$  and  $e_c$  are strains perpendicular to the  $c$  axis and parallel to it, respectively. The hydrostatic uniaxial pressure derivative of  $T_C$  in the hexagonal structure can be written [17]

$$dT_C/dP = 2(\partial T_C / \partial e_a)(de_a/dP) + (\partial T_C / \partial e_c)(de_c/dP). \quad (2)$$

We obtain the following relation:

$$dT_C/dP = 2dT_C/dP_a + dT_C/dP_c \quad (3)$$

on the assumption that the uniaxial pressure derivative  $dT_C/dP_L$  ( $L = a, c$ ) of  $T_C$  is defined as

$$dT_C/dP_L = (\partial T_C / \partial e_L)(de_L/dP).$$

The magnitude of  $dT_C/dP_L$  ( $L = a, c$ ) in (3) is estimated by using the Ehrenfest relation for the  $a$  and  $c$  axes:

$$dT_C/dP_L = T_C V_{\text{mol}} \Delta\alpha_L / \Delta C_p. \quad (4)$$

Since  $\Delta\alpha_L$  ( $L = a, c$ ) and  $\Delta C_p$  are negative and positive, respectively,  $dT_C/dP_L$  ( $L = a, c$ ) are also negative. Then,  $dT_C/dP$  remains large and negative. However, as  $\delta$  increases beyond  $\delta = 0.33$ ,  $\Delta c$  tends to be tiny or nearly zero [8, 11]. As a result, the second term  $dT_C/dP_c$  in (3) is eliminated when  $\delta = 0.33$  ( $\text{Cr}_2\text{Te}_3$ ), i.e.  $dT_C/dP_c$  is equal to  $2dT_C/dP_a$ .



Equation (3) for  $\delta = 0$  (CrTe) and  $\delta = 0.33$ , ( $\text{Cr}_2\text{Te}_3$ ), respectively, are expressed as follows:

$$(dT_C/dP)_{\delta=0} = 2(dT_C/dP_a)_{\delta=0} + (dT_C/dP_c)_{\delta=0} \quad (5)$$

$$(dT_C/dP)_{\delta=0.33} = 2(dT_C/dP_a)_{\delta=0.33}. \quad (6)$$

Since  $\Delta a$ , as a measure of  $\Delta\alpha_a$ , is nearly independent of  $\delta$ , it follows that  $(dT_C/dP_a)_{\delta=0} = (dT_C/dP_a)_{\delta=0.33}$ , taking account of (3). Then, we subtract (6) from (5), to obtain

$$(dT_C/dP)_{\delta=0} - (dT_C/dP)_{\delta=0.33} = (dT_C/dP_c)_{\delta=0}. \quad (7)$$

If one subtracts  $(dT_C/dP)_{\delta=0.33} = -1.78 \text{ K kbar}^{-1}$  [11] from the present value of  $(dT_C/dP)_{\delta=0}$ , the right-hand side in (7) is found to be  $-5.22 \text{ K kbar}^{-1}$ . The value of  $(dT_C/dP_c)_{\delta=0}$  is determined as  $-5.7 \text{ K kbar}^{-1}$ , substituting  $\Delta\alpha_c = -5.6 \times 10^{-5} \text{ K}^{-1}$ ,  $\Delta C_p = 18.03 \text{ J mol}^{-1} \text{ K}^{-1}$  [16],  $V_{\text{mol}}(T = T_C) = 52.13 \text{ cm}^3 \text{ mol}^{-1}$  and  $T_C = 350 \text{ K}$  in (4). This value is in good agreement with the value of  $-5.22 \text{ K kbar}^{-1}$  estimated using (7). From this estimate, it seems that the anomalous  $\delta$  dependence of  $dT_C/dP$  in the  $\text{Cr}_{1-\delta}\text{Te}$  system originates from the increase in  $dT_C/dP_c$  as  $\delta$  increases from 0 to 0.33.

The pressure derivative of  $T_C$  is related to the magnetic Grüneisen parameters  $\gamma_M$  [18] which is defined by

$$\gamma_M = B_C (d \ln T_C) / dP = -d(\ln T_C) / d\omega. \quad (8)$$

Here,  $B_C$  is the bulk modulus at  $T_C$  which is equal to the reciprocal of the compressibility  $\kappa$ . The volume bulk modulus  $B$  is evaluated to be  $6.02 \times 10^2 \text{ kbar}$  using the smoothed values [5] of  $a/a_0$  and  $c/c_0$  at room temperature, where  $a_0$  and  $c_0$  are the values of  $a$  and  $c$ , respectively, at ambient pressure. If  $B$  is assumed to be approximately equal to  $B_C$  since the difference between  $T_C$  and room temperature is small,  $\gamma_M$  is determined to be 12.04, substituting  $dT_C/dP = -7.0 \text{ K kbar}^{-1}$ ,  $T_C = 350 \text{ K}$  and  $B = 6.02 \times 10^2 \text{ kbar}$  in (8). The value obtained for  $\gamma_M$  is consistent with the previous result ( $\gamma_M = 8 \pm 1.5$ ) [19]. On the basis of the uniaxial pressure derivatives derived in the preceding paragraph, the orientation-dependent magnetic Grüneisen parameter  $\gamma_M^L$  ( $L = a, c$ ) for the  $a$  and  $c$  axes is defined as

$$\gamma_M^L = B_C^L (d \ln T_C) / dP_L = -d(\ln T_C) / d\omega_L \quad (9)$$

using the value of  $dT_C/dP_L$  and the uniaxial bulk modulus  $B_C^L$  at  $T_C$ . From the values [5] of the uniaxial compressibilities  $\kappa_a = 4.1 \times 10^{-4} \text{ kbar}^{-1}$  for the  $a$  axis and  $\kappa_c = 8.4 \times 10^{-4} \text{ kbar}^{-1}$  for the  $c$  axis at room temperature, the values of  $B^L$  ( $L = a, c$ ) are calculated to be  $B^a = 1.19 \times 10^3 \text{ kbar}$  and  $B^c = 2.44 \times 10^3 \text{ kbar}$ , respectively. The values of  $\gamma_M^a$  and  $\gamma_M^c$  are determined to be 6.20 and 17.75, respectively, substituting  $(dT_C/dP_a)_{\delta=0} = -1.78 \text{ K kbar}^{-1}$ ,  $(dT_C/dP_c)_{\delta=0} = -5.22 \text{ K kbar}^{-1}$ ,  $B^L$  ( $L = a, c$ ) and  $T_C = 350 \text{ K}$  in (9). Here,  $B^L$  ( $L = a, c$ ) is also assumed to be approximately equal to  $B_C^L$ . It may be noted that the magnitude of  $\gamma_M^c$  is about three times that of  $\gamma_M^a$ .

For supplementary information, the thermal expansion anomalies are observed in the temperature range far below and above  $T_C$ . Firstly, a strong contraction of both  $a$  and  $c$  is observed around 600 K where the break in the  $\chi^{-1}$  versus  $T$  curve also occurs. From the measurement of the heat capacity for CrTe [14], the endothermic reaction has been observed around 600 K. At this temperature, CrTe decomposes into CrTe,  $\text{Cr}_3\text{Te}_4$  and  $\text{Cr}_2\text{Te}_3$ , as

confirmed by x-ray diffraction [14]. This decomposition temperature is compared with the temperature where the second strong contraction in the  $a$  and  $c$  versus  $T$  curves is observed in the present study. Therefore, a drastic change in both  $a$  and  $c$  around 600 K suggests that CrTe decomposes into other phases. Secondly, below about 150 K,  $a$  increases on cooling to 15 K, while  $c$  monotonically decreases. In order to consider this behaviour, more detailed experiments at low temperatures will be necessary. Thirdly, it is important to point out the empirical relation between the band structure and the thermal expansions in the  $\text{Cr}_{1-\delta}\text{Te}$  system. The values of  $\Gamma^s$  ( $s = +, -$ ) are plotted against  $\delta$  in figure 5. Here,  $\Gamma^s$  ( $s = +, -$ ) is a normalized partial density of states in the ground state, defined as

$$\Gamma^s = N^s(E_F)/N_{\max}^s(E)$$

where  $N^s(E_F)$  ( $s = +, -$ ) are the partial densities of states for the majority and minority spins, respectively, at Fermi level  $E_F$ , calculated in [20] and  $N_{\max}^s(E)$  is the maximum value of  $N^s(E)$  at energy  $E$ . From this figure,  $\Gamma^+$  remains nearly constant, while  $\Gamma^-$  decreases from about 0.2 for  $\delta = 0$  (CrTe) to zero for  $\delta = 0.33$  ( $\text{Cr}_2\text{Te}_3$ ) with increasing  $\delta$ . It should be noted that the  $\delta$ -dependences of  $\Delta L$  ( $L = a, c$ ) correspond well to those of  $\Gamma^s$  ( $s = +, -$ ). It is probable that these situations are related to the different thermal expansion anomalies for the  $a$  and  $c$  axes observed experimentally in the  $\text{Cr}_{1-\delta}\text{Te}$  system.

## 5. Conclusions

The present investigation of the pressure effect and the thermal expansion for CrTe, together with the reported data for  $\text{Cr}_{1-\delta}\text{Te}$  ( $0 < \delta \leq 0.35$ ), discloses the following features. A large negative pressure derivative of  $T_C$  in CrTe is observed. From the linear forced magnetostriction, the spontaneous magnetization depends on the volume even at 4.2 K. Thermal expansion anomalies in both  $a$  and  $c$  are observed below  $T_C$ . The value of  $q_c/q_s$  in the interval  $380 \text{ K} < T < 600 \text{ K}$  is found to be 1.3. These features indicate that CrTe can be classified as an itinerant ferromagnet. The uniaxial pressure derivative of  $T_C$  gives a large magnetic Grüneisen parameter for the  $c$  axis, compared with that for the  $a$  axis when a bulk modulus at room temperature is assumed. The observed anomalous behaviour of  $dT_C/dP$  as a function of  $\delta$  in the  $\text{Cr}_{1-\delta}\text{Te}$  system may be due to the strong increase in the uniaxial stress derivative of  $T_C$  along the  $c$  axis as  $\delta$  increases.

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