Incommensurate phase transition in $TlGaTe_2$

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(Submitted 18 March 1987)
Pis'ma Zh. Eksp. Teor. Fiz. **45**, No. 9, 418–420 (10 May 1987)

A phase transition in layered $TlGaTe_2$ chain crystals has been observed for the first time at $T = 98.5$ K. Structural features characteristic of an incommensurate phase have also been observed.

1. The $TlGaTe_2$ crystal is a semiconductor that belongs to a group of strongly anisotropic TlSe-type chain semiconductors which have several interesting physical properties. The band structure of $TlGaTe_2$ was calculated in Refs. 1 and 2 on the basis of crystal-structure data of Ref. 3. The possibility that TlSe crystals can have second-order phase transitions was theoretically predicted in Ref. 4. In the present letter we present the results of x-ray diffraction and calorimetric experiments and also the results of measurements of the electrical conductivity in the study of the phase transition and modulated structures in $TlGaTe_2$.

2. The x-ray diffraction studies were carried out using DRON-3 (CuK_α radiation) with a low-temperature attachment URNT-180. The temperature was measured in 5-K steps. The lattice parameters of $TlGaTe_2$ are $a = 8.429$ Å, $c = 6.865$ Å, and space group[3] $I4/mcm - D_{4h}^{18}$. A detailed x-ray diffraction study of $TlGaTe_2$ crystals revealed an unusual temperature behavior of the lattice parameters. The temperature dependence of the parameter a (curve 1 in Fig. 1) revealed the presence of several invariant regions (110–160 K, 180–210 K, 240–270 K) between which the parameter a increased monotonically. The $a(T)$ curve exhibits a strong anomaly in the temperature interval 90–110 K.

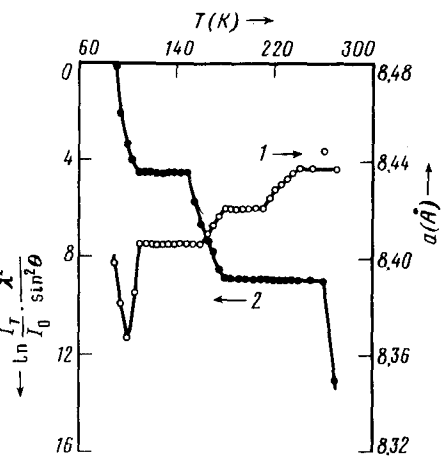

FIG. 1 Temperature dependence of the lattice parameter a (1) and $\ln(I_T/I_{90})(\lambda^2/\sin^2\theta)$ (2) in $TlGaTe_2$.

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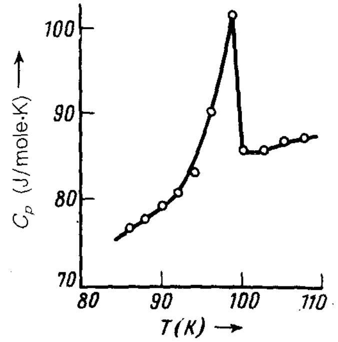

FIG. 2. Temperature dependence of the specific heat of $TlGaTe_2$ in the region of the anomalies.

The intensities of the Bragg reflections (200) and (211) were measured in the temperature range under study. The results of measurements of the (200) reflection are shown on curve 2 in Fig. 1. The plot shows that the intensity of the diffraction reflections correlates well with the $a(T)$ dependence. A similar temperature behavior of the lattice parameters and of the intensity of the x-ray reflections was observed previously in ZnP_2 (Refs. 5 and 6), $NaNO_2$ (Ref. 7), and $(NH_4)_2BeF_4$ (Ref. 8). The authors of Ref. 6 attributed the results obtained by them to the existence of a complete devil's staircase.

3. We have measured the heat capacity (C_p) in the temperature interval 5–300 K in an adiabatic calorimetric apparatus with an automatic temperature control. The results of the calorimetric studies were reported in part in Ref. 9. In the anomalous regions of $a(T)$ we carried out several additional sets of measurements, varying the temperature steps. Figure 2 shows the results of one of these measurements. In the $TlGaTe_2$ sample the $C_p(T)$ curve exhibits a structural feature at 98.5 K. We also see on this curve a finite jump in the heat capacity on the order of 20% of its value near the jump. In the vicinity of the jump, the entropy and enthalpy change by the amount 0.61 J/mole·K and 58.6 J/mole, respectively. The structural feature which is observed depends on the steps at which the temperature was measured and on the heating-cooling cycle for the repeated measurements. Latent heat evolution was not detected.

4. We have also measured the temperature dependence of the conductivity (σ) in order to determine the effect of the phase transition on the electron subsystem of the $TlGaTe_2$ crystals. The measurements were carried out in the direction of the cooling. An anomalous region of $\sigma(T)$ is observed near 93 K. The magnitude of the jump is 38%.

Taking all the results into account, we conclude that (a) at 98.5 K the $TlGaTe_2$ crystals undergo a second-order phase transition, (b) the thermal behavior of the lattice parameter and of the intensity of the Bragg reflection in the temperature region 110–290 K is similar in nature to the periodic modulation characteristic of an incommensurate phase.[10,11] A definitive resolution of the question regarding the nature of the phase transition at 98.5 K and the reason for the appearance of an incommensurate phase requires, however, further comprehensive study.

We wish to thank F. M. Gashimzade for a useful discussion and for pointed remarks.

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Translated by S. J. Amoretty