PROPERTIES OF $NbTe_4$ AND $TaTe_4$

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Temperature dependence of the electrical resistivity, its anisotropy and thermoelectric power are reported of $NbTe_4$ and $TaTe_4$, 1/3-filled charge density wave systems.

1. Introduction

In the tetragonal tetratelluride of Nb and of Ta, linear chains of equi-distant metal atoms are centered in the channels formed by Te square antiprisms.[1,2] $TaTe_4$ shows the commensurate modulation (2a,2a,3c) at room temperature; Ta atoms show a longitudinal periodic displacement with the period of (3/2)c (forming triple Ta clusters)[3]. In $NbTe_4$[4-7], the room temperature phase is incommensurate with the wave vector $(2/3+\delta)c^*$,where $\delta = 0.022$ [8]. On cooling below 180K, the transverse period is changed from $\sqrt{2} \times \sqrt{2}$ to 2 x 2 and the modulation becomes discommensurate with the period of 16(c/2). At 50K it locks into the commensurate $TaTe_4$ structure.

2 Experimental results and discussion

Single crystals of $TaTe_4$, prepared by the iodine transport, show the residual resistance ratio R(300K)/R(4K) (RRR) between 50 and 200. $NbTe_4$ crystals were grown under various conditions in Lausanne.

Of both $NbTe_4$ and $TaTe_4$, the resistivity along the c-axis, ρ_c is (0.5- 2) $10^{-4}\,\Omega$cm at room temperature. Figure 1 shows ρc and its temperature derivative $d\rho c/dT$ of $TaTe_4$. Because the lock-in transition temperature is well above 300K, no structure is found in the resistivity. The ratio $\rho c/\rho a$ is equal to 1, between 4K and 300K; the Peierls transition temperature is high

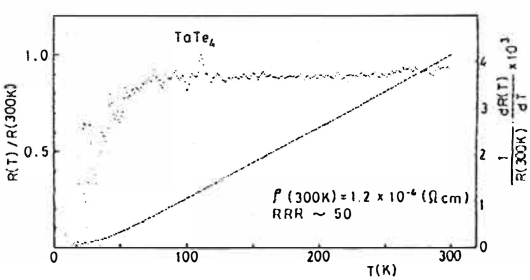

Fig.1 Resistivity along the c-axis and its temperature derivative of $TaTe_4$

and the remaining Fermi surface is much more isotropic. Figure 2 shows examples of the measured resistivity of $NbTe_4$. A change of its temperature derivative is found at 50K, which is indicative

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of a larger resistivity below 50K than that extrapolated from above. At 200K a cusp is observed which corresponds to the change in the transverse periods. The resistivity change at the transition temperatures is similar to those observed at the CDW transition temperatures in, e.g., $NbSe_3$, but the increment is much smaller. The resistivity is isotropic in the a-c plane in the whole temperature range. No change in $\rho c/\rho a$ is found at the transition temperatures; it shows only a slight increase with lowering temperature. This suggests that no anisotropic scattering mechanism is associated with the CDW structural change.

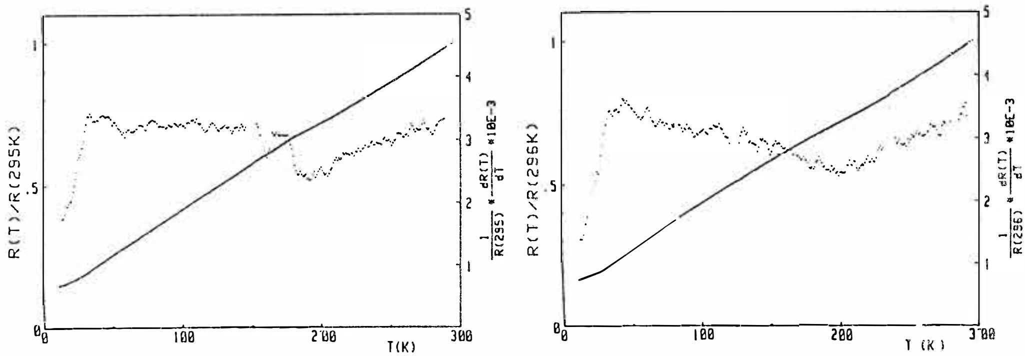

Fig. 2 Resistivity and its temperature derivative of $NbTe_4$, of "good quality (a) and of "poor" one (b).

All crystals of $NbTe_4$ examined so far showed poor residual resistance ratio of less than 10, irrespective of growth condition. As far as examined, the purity of Nb and Te has no relation to the quality of the products. It is probable that crystals is Te-deficit; lower growth temperature results relatively larger RRR values, in general. Another possibility is that the transport agent, iodine or chlorine, is incorporated as randomly distributed impurity or these atoms are trapped at defects of the CDW structure during crystal growth.

Two types of resistivity change at 200K are observed, as shown in Fig.2. Crystals of relatively larger RRR show a clear cusp at 200K and ρc is linear above 50K, while in those of poorer RRR the cusp at 200K is less clear and $d\rho c/dT$ shows a gradual change with temperature above 50K; the change at 200K is more sluggish, without temperature hysteresis, presumably because rich defects/impurities work as barriers against the CDW phasing. It is rather surprising that small differences of RRR are correlated to observable difference in physical properties.

The thermoelecric power S(T) of $NbTe_4$ parallel to the c-axis is shown in Fig.3. The lock-in transition is clearly revealed. The change at 200K is less clear but a change in the slope is found in a sample grown in liquid Te, which shows clearer resistivity change. Zero crossing is found slightly above room temperature.

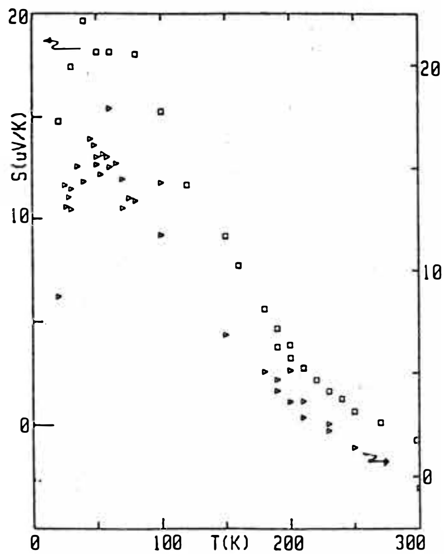

Fig.3 Thermo-electric power of $NbTe_4$ (square:grown from liquid Te, triangle:Nb-excess)

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