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Electronic structure and transport properties of uniaxially deformed m - TaS₃

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Abstract

Due to relative simplicity of its crystal and electronic band structure, apparent absence of any temperature or strain induced commensurate-incommensurate transitions monoclinic (m-) TaS₃ may be regarded as a parent compound for the whole family of transition metal trichalcogenides. In present work an attempt is made to relate the recently obtained results in studying electronic properties of uniaxially deformed m-TaS₃ [1] with the band-structure calculation [2].

Introduction

The peculiarity of m-TaS₃ crystal structure [3] is the existence of nearly "isolated" chains denoted as type III, and type I chains, which are connected to type II chains via relatively short S-S distance (comparable to that within trigonal prisms).

According to band structure calculations [2] electronic structure of m-TaS₃ is presented by four nearly quarter-filled bands with a very similar dispersion along Γ -Y direction and slightly shifted in energy (bands a in fig. 1).

Fig.1. Band structure of m-TaS₃ from ref. [2].

Fig.2. The thermopower vs inverse temperature. Inset the behavior of thermopower in a vicinity of T_{p2} is shown.

Two Fermi surface (FS) sheets originated from type III chains are almost flat, while those produced by type I are essentially wrapped due to well pronounced dispersion along Γ -X direction attributed to a strong inchain interaction between type I and type II chains.

The main features, observed in experiments with uniaxial strain deformation

The electronic properties of m-TaS₃ have been studied in 80-300 K temperature range under uniaxial stretch deformation $S=1-2\%$. The details of experimental technique are described elsewhere [1]. Here we summarize the main observations of [1] for the purpose of further discussion.

At $T > T_{P1}$ (240 K) the conduction has a metallic character with a weak strain dependence and negative sign of thermopower.

Between T_{P1} and T_{P2} (160 K) the conduction is nearly temperature independent. At T_{P1} the thermopower changes its sign to a positive one and becomes again negative in a vicinity of T_{P2} (Fig 2). The sign of thermopower is also changed to a negative under a strain deformation (Fig 3b).

Fig.3. The strain dependence of thermopower for m-TaS₃.

At $T < T_{P2}$ the conductivity is characterized by a well defined activation law. A strong strain dependence of conductivity is observed (Fig. 4), while thermopower remains almost strain independent (Fig. 3a). The apparent meaning of E_g is not affected by strain.

Uniaxial deformation lowers T_{P2} , while leaves T_{P1} nearly unaltered (Fig. 5).

The role of transversal contraction

From a comparison of our data on the strain dependence of electronic properties of m-TaS₃ with results of studying its properties under hydrostatic pressures [4,5] one may conclude, that a transversal contraction of uniaxially stretched samples is playing an important and sometimes dominant role.

The conduction of m-TaS₃ grows approximately 2 times both under uniaxial strain deformation of order 2% and under hydrostatic pressure of 10 kbar [4] as well. Taking for a rough estimate a Young module of m-TaS₃ to be equal to that of o-TaS₃, and proposing the anisotropy of Young module to be of order of 10, we obtain, that a transversal contraction of a sample under pressure of 10 kbar is approximately the same, as under a strain deformation of order 2%. Therefore, irrespective of a mechanism of conduction growth (discussed in more details below) one may conclude that a transversal contraction is playing a dominant role.

T_{P2} is lowered both under strain deformation and under pressure, showing that a transversal contraction plays a leading role.

T_{P1} remains nearly unaltered in our experiments, while a weak non-monotonic strain dependence of T_{P1} was observed in [6]. This means, perhaps, that in the case of nearly flat FS the

Fig.4. The strain dependence of conduction for m-TaS₃ at various temperatures. Conduction is normalized to its own value at zero strain and the same temperature. Raw data used for evaluation of this surface are the same as in fig. 2 of ref. [1].

role of transversal contraction is small, and the effect of sample elongation and transversal contraction are comparable.

The high-temperature transition

According to [2] a high-temperature transition (240 K) is attributed to FS sheets associated mainly with type III chains. These bands are slightly more than quarter-filled and appropriate superlattice is characterized by $Q = \{0, 0.255, 0\}$. At $T > T_{P1}$ the conduction should have electronic nature in accordance with the observed sign of thermopower. After a superlattice formation at T_{P1} the small hole pockets are formed at a new zone boundary in of other bands, lying higher in energy. This picture is confirmed by observed change of thermopower sign near T_{P1} .

The bands are characterized by nearly flat FS sheets providing a good nesting conditions resulting in high T_P . Due to essentially small dispersion along Γ -X and Γ -Z directions such FS should be insensitive to transversal contraction. Indeed, T_{P1} is nearly unaltered by strain deformation.

The low-temperature transition

Within a band structure [2] a low temperature transition (160 K) is attributed to FS sheets originated primary from type I chains. These bands are higher in energy and hence less than quarter-filled. The appropriate observed superlattice has an Y component 0.245 c.

Due to strong interaction between type I and type II chains a strong dispersion along Γ -X direction arises with a result that FS sheets are essentially buckled. Appropriate nesting condition occurs for superlattice with $Q = \{0.5, 0.245, 0.5\}$. Within this picture lowering of T_{P2} both under hydrostatic pressure and uniaxial strain deformation is attributed to a progressively growing of Γ -X dispersion due to transversal contraction with the result that nesting becomes impeded.

A Peierls gap of m-TaS₃

There is an obvious contradiction between an apparent strain independence of activation energy (see Fig.4) and lowering of T_{P2} under strain deformation. This contradiction is tightly related to a problem of the origin of conduction growth under a strain deformation.

First, it should be mention, that according to [2] the energy shift between the bands in o-TaS₃ is lower, or at least comparable to the Peierls gap. In this case the value of a gap, obtained from temperature dependence of conduction and the amplitude of the order parameter do not always coincide [7]. A criterion for this coincidence, based on the estimation of a gap, induced by a Peierls transition in one of bands, in other bands, is very difficult to check experimentally. Another source of uncertainty come from a well known fact, that experimentally observed T_P is really a temperature of 3D ordering, and not a mean-field Peierls temperature. Therefore, we believe, that the transport measurements give a more appropriate base for a gap estimation, then the changes of T_P .

Fig.5. The logarithmic derivative of resistivity.

Fig.6. The nonlinear conductivity vs electric field for m-TaS₃ at 90 K. Field is normalized to E_t .

From that point of view, a rise of conduction in m-TaS₃ under a strain deformation (and under a hydrostatic pressure as well) is attributed rather to a growth of carrier mobility, then to diminishing of a Peierls gap.

This conclusion is reenforced by absence of remarkable changes of thermopower under strain sufficient to be responsible for observed growth of conduction. Moreover, lowering of the order parameter amplitude would lead to diminishing of a threshold field which is in contradiction with the experiment.

Comments on dynamics of CDW in m-TaS₃

In most Linear chain compounds a dynamics of CDW is well described within a model taking in account the effects of screening charged CDW deformations by free carriers [8,9]. A most complete set of data was collected for K_{0.3}MoO₃, and it was shown, that proportionality between σ_{CDW} and σ_{el} is retained when a free carrier concentration is changed by temperature [10] or pressure application [11].

In m-TaS₃ the field dependence of non-linear conduction show an universal strain independent behavior with E_t being the only scaling parameter (Fig.6). Such a behavior seems to contradict the predictions of screened CDW dynamics model because the non-linear conduction is not changed, when a linear conduction grows two times under deformation. For that reason mechanisms other than free carrier dumping should be regarded for m-TaS₃.

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