

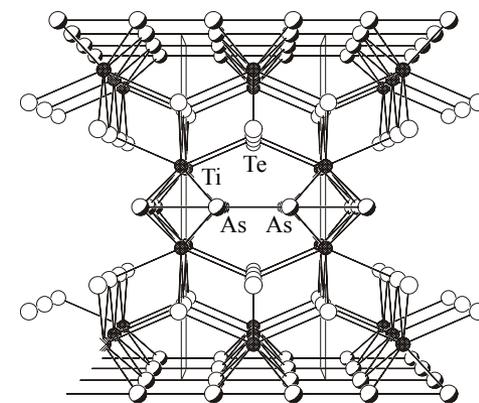
Synthesis, Structure, Electrical Properties, and Band Structure Calculations of TiAsTe

James A. Ibers, Northwestern University, DMR-0096676

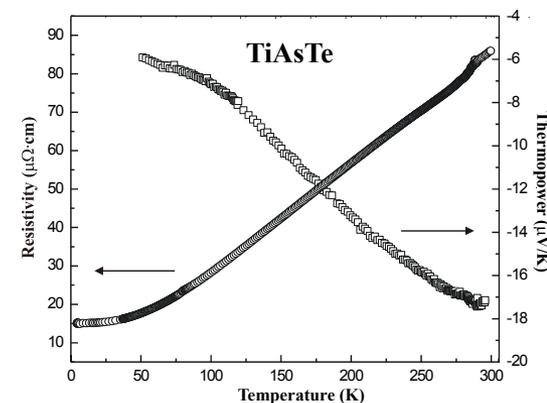
Collaborators: Fu Qiang Huang, Christine Flaschenriem, Paul Brazis, Carl R. Kannewurf

TiAsTe has been synthesized by the reaction of the elements at 923 K. Its structure is of the NbPS type and contains linear infinite As chains. On the basis of the As-As bond lengths the formal oxidation states may be taken as intermediate, namely $3 + \square$ for Ti, $-(1 + \square)$ for As, and -2 for Te, with $0 < \square < 1$. The resultant compound is an n-type metal. Density functional theory calculations help rationalize the chemical bonding and physical properties.

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Structure of TiAsTe



Electrical resistivity and thermopower vs. temperature

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Education:

Christine Flaschenriem, the graduate student on this project, is now a Crystallographic Specialist at the University of Rochester; Paul Brazis, a graduate student with Prof. Carl R. Kannewurf in the Electrical and Computer Engineering Department, is now with Motorola Corporation; Fu Qiang Huang, a postdoctoral on this project, is now at the University of Pennsylvania.

Impact on Other Areas:

This study has led to an understanding of the differences in some of the physical properties of NbPS, NbPSe, and TiAsTe as a group V metal (Nb) is replaced by a group IV metal (Ti). Such an understanding will help in the design of new materials displaying important metallic conductivity and thermoelectric properties.