High-Pressure Crystallographic Study of SnS_2 and TiS_2

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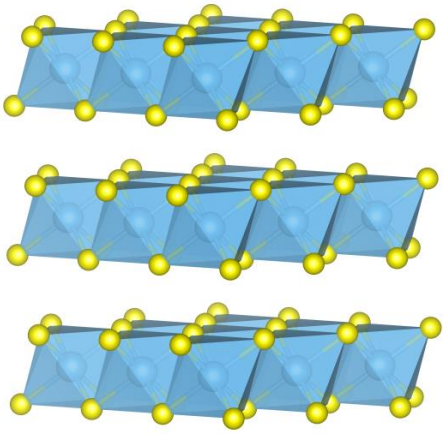
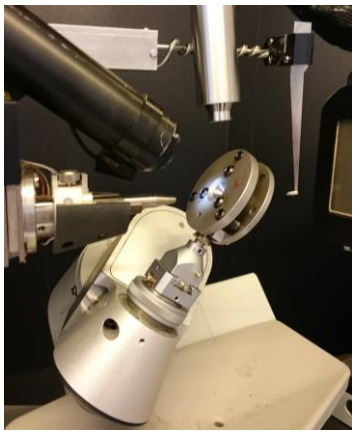
The applications of layered disulfides are vast and range from lubricants[1] and electrode materials[2] to optoelectronic devices and transistors.[3] The interesting electronic properties are intimately related to the atomic structure seen below, in particular the S-S interlayer interactions.

So what happens to these very interactions when the layers are forced closer together? In this study, pressures up to 20 GPa are applied to single crystals of SnS_2 and TiS_2, synthesized and grown in our own labs. The crystal is mounted in a Diamond Anvil Cell, as seen in the picture below, and X-ray diffraction is utilized to thoroughly analyze the atomic and electronic structure changes of SnS_2.





The stunning and very pronounced change in physical appearance is directly linked to the change in electronic structure. Isostructural compounds have been found to undergo a semiconductor -> semimetal transition,[4] but this transition has never before been documented for SnS_2.

In contrast, TiS_2 is found to be a semimetal at ambient pressures.[5] Much more interesting is a reported phase transition around 16 GPa found through theoretical calculations,[6] but never before confirmed through experiment.

The goal of this analysis is, along with further experiments, to expand the knowledge of the S-S interlayer interaction and its impact on the structural and electronic changes caused by pressure. Expanding the knowledge on these compounds is an important step towards further utilization in advanced applications.

1. Martin, J.; Donnet, C.; Le Mogne, T.; Epicier, T., *Phys. Rev. B,* **1993**. 48, 10583-10586
2. Scrosati, B., *Nature,* **1995**. 373, 557-558
3. Radislavljevic, B.; Radenovic, A.; Brivio, J.; Giacometti, V.; Kis, A., *Nat. Nanotechnol.* **2011**. 6**,** 147-150
4. Allan, D. R.; Kelsey, A. A.; Clark, S. J.; Angel, R. J.; Ackland, G. J., *Phys. Rev. B,* **1998.** 57, 5106-5110
5. Liu, B.; Yang, J.; Han, Y.; Hu, T.; Ren, W.; Liu, C.; Ma, Y.; Gao, C., *J. Appl. Phys.* **2011**. 109, 05371
6. Yu, Y. G.; Ross, N. L., *J. Phys.: Condens. Matter,* **2011**. 23, 055401