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The effect of sample purity on the charge density wave compound TiSe₂

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We have investigated the electronic structure of the charge density wave (CDW) compound TiSe₂ using detailed X-ray photoelectron spectroscopy (XPS) measurements from the core levels (Ti 2p, Se 3p and Se 3d), as well as the valence band. Four different samples were provided to us by collaborators at the University of Bath, in addition to corresponding resistivity measurements. Each batch has different sample purity and thus stoichiometry, due to different growth conditions. The four samples were studied in their cleaved and uncleaved forms, after which they were stored in air and reinvestigated. XPS data were obtained at room temperature using two different photon energies (hnu; = 1486.71 eV and 2984.3 eV), so that the contribution to the electronic structure of both the surface and bulk of the samples could be probed.
It was found that the cleanliness of the sample surface lasts for approximately 24 hours with minimal contamination in vacuum, and that air storage affects the contamination to a large degree. Using the data obtained, the Ti:Se stoichiometry of each sample was determined. These results were compared to the transport properties measurements provided. As expected, the resistivity depends largely on the growth conditions – hence the sample purity. The resistivity curve of the purest sample batch peaks at a critical temperature of 202 K, which corresponds to the CDW transition temperature. When comparing the stoichiometry found using XPS to the resistivity curve, it was found that a deviation of 5-10 % from the 1(Ti):2(Se) expected stoichiometry resulted in a lowering of the CDW transition temperature to 125 K. So in agreement with the expected results, the more pure the sample was found to be, the closer the peak in the resistivity is to the maximum CDW transition temperature.
In the future we will use angle resolved photoelectron spectroscopy in order to investigate the effect of stoichiometry and sample purity on the low-energy electronic structure features displayed by the same samples. We foresee that this will shed light on the controversial debate on the structure of the CDW phase reported for TiSe₂ and the fact that that it may be a 2x2x1 structure as opposed to the previously assumed 2x2x2 structure.

Summary

The electronic structure of the charge density wave (CDW) compound TiSe₂ using detailed X-ray photoelectron spectroscopy (XPS) measurements from the core levels (Ti 2p, Se 3p and Se 3d), as well as the valence band. Four different samples, each with different purity and stoichiometry, were provided to us by collaborators at the University of Bath, in addition to corresponding resistivity measurements. XPS data were obtained at room temperature using two different photon energies (hnu; = 1486.71 eV and 2984.3 eV).
It was found that the cleanliness of the sample surface lasts for approximately 24 hours with minimal contamination in vacuum, and that air storage affects the contamination to a large degree. The Ti:Se stoichiometry of each sample was determined and the results compared to the transport properties measurements provided. The resistivity depends largely on the growth conditions – hence the sample purity. The resistivity curve of the purest sample batch peaks at a critical temperature of 202 K, which corresponds to the CDW transition temperature. When comparing the stoichiometry found using XPS to the resistivity curve, it was found that a deviation of 5-10% from the 1(Ti):2(Se) expected stoichiometry resulted in a lowering of the CDW transition temperature to 125 K. So in agreement with the expected results, the more pure the sample was found to be,

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