Why the phase-change material iron-tellurium best conducts electricity in its disordered amorphous phase

October 7 2016

Solid materials whose atoms are arranged in a well-ordered crystalline structure are usually better conductors of electricity than randomly structured, or amorphous, solids. Recently, however, A*STAR researchers found that iron-tellurium (FeTe) breaks this rule, displaying higher conductivity, and optical reflectivity, in the amorphous phase.

A recent study, published in the journal Acta Materialia, describes their efforts to understand why FeTe's behavior is counterintuitive to expectations.

FeTe is a phase-change material, with the ability to rapidly switch its state from crystalline to amorphous and back again when it is heated or cooled, a property which makes it useful for data storage and memory applications. Conventional phase-change materials such as germanium-antimony-tellurium (GST), commonly used in rewritable DVDs, display higher optical reflectivity and electrical conductivity in their crystalline state because the highly-ordered structuring of atoms in the crystal results in more electron vacancies, or holes, that act as charge carriers.

"FeTe behaves differently from other phase-change materials," explains Kewu Bai at the A*STAR Institute of High Performance Computing, who worked on the project with scientists from the National University of Singapore. "We hypothesized that these unusual characteristics may be connected with the behavior of 'lone-pair' electrons. This refers to a pair of electrons from any one atom that are not involved in the bonding of materials."

The team prepared thin films of FeTe at room temperature to produce amorphous structures, and at 220 degrees Celsuis to acquire crystalline samples, and showed that the films could be flipped between the two states using a fast pulsing laser. They analyzed the molecular structure of the different films using X-ray spectroscopy, electron microscopy and first-principle calculations to investigate these unusual properties of FeTe.

The researchers confirmed the existence of lone-pair electrons in both the amorphous and crystalline phases. In the crystalline phase, where Te and Fe atoms were strongly bonded in a regular lattice, electrons were engaged in strong hybridization, meaning their orbitals overlapped and caused their electrons to localize. Thus, lone-pair electrons were incorporated as part of the integral structure.

In contrast, when FeTe entered its amorphous phase, some Te atoms were orientated so that their lone-pair electrons delocalized from the atoms, resulting in holes that acted as charge carriers.

"We are hopeful that FeTe could prove to be useful material for phase-change memory," says Bai. "It could also act as an effective thermo-electric material, generating electric current in response to temperature."

More information: H.W. Ho et al. Unravelling the anomalous electrical and optical phase-change characteristics in FeTe, *Acta Materialia* (2016). DOI: 10.1016/j.actamat.2016.04.017

Provided by Agency for Science, Technology and Research (A*STAR),

Singapore

Citation: Why the phase-change material iron-tellurium best conducts electricity in its disordered amorphous phase (2016, October 7) retrieved 21 June 2024 from https://phys.org/news/2016-10-phase-change-material-iron-tellurium-electricity-disordered.html