PRESS RELEASE

Penetrable barriers – tunnelling welcome

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The boundaries between grains in certain thin-film materials are no obstacle to charge carriers. They even help prevent losses in charge transport. Researchers from Helmholtz-Zentrum Berlin obtain experimental evidence for a bold theory.

A solar cell is quite simple in principle: Incident sunlight releases charge carriers inside a light-absorbing material, and these charge carriers move towards connected contacts. But in reality, there are complications. The charge carriers have to overcome a number of obstacles in their path. Getting these obstacles out of the way is one of the main concerns of photovoltaic research. Now, researchers at Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) have solved an important, fundamental physical problem that arises in the design of latest generation thin-film solar cells. Their solution will appear in the coming issue of Physical Review Letters.

Inside polycrystalline materials, which are made up of many tiny crystals known as grains, the boundaries between grains present obstacles. Despite this, it has been observed that the monocrystalline form of certain copper minerals (chalcopyrite) is actually much worse at conducting electricity than polycrystalline forms with their many grain boundaries. Michael Hafemeister and Sascha Sadewasser of HZB together with Susanne Siebentritt of the University of Luxembourg have managed to explain why this is so. They have demonstrated that an electric barrier forms at each of the grain boundaries, and that the charge carriers can tunnel through these barriers thanks to their quantum mechanical behaviour.

“An American research group predicted the existence of such a barrier in chalcopyrites using computer simulations as far back as 2003. Now we have shown in our experiment that this barrier does indeed exist,” explains Sascha Sadewasser.

They did so by performing an experimental trick: Michael Hafemeister and his colleagues grew a chalcopyrite crystal (copper-gallium-diselenide) in the form of a crystal pair. To do this, they took a gallium-arsenide crystal consisting of two large grains as a substrate, and vapour-deposited a layer of chalcopyrite onto it. As the layer grew, it adopted the structure of the gallium-arsenide crystal, thus providing a model system with a perfectly defined grain boundary. Employing a whole battery of elaborate measuring techniques, the physicists investigated the boundary and the behaviour of electric charge carriers at the boundary. One of the things they investigated – for the first time – was the electrical resistance between the crystals, where they discovered that a barrier of about half an electron volt drastically retards the flow of current.

With the results of this measurement, it was certain: “Without the barrier, the electrical resistance under the given physical conditions would have to have been lower,” says Sascha Sadewasser. This means that, while the barrier is an obstacle to electrical conductivity, it also prevents too many charge carriers – negatively charged electrons and positively charged atomic cores (holes) – from recombining on the spot. “There are of course many positive charge carriers in the chalcopyrites. The barrier makes sure they don’t hang around near the border. That prevents the oncoming free electrons produced

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by light incidence from being captured," explains Sadewasser. Nevertheless, the current flow still works, as the electrons can tunnel through the barrier.

Good current flow despite many grain boundaries – the secret of polycrystalline chalcopyrites has thus been revealed. And with this knowledge, perhaps we can modify the grain boundaries to the right properties to increase the efficiency of solar cells that little bit further.

The **Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)** operates and develops large scale facilities for research with photons (synchrotron beams) and neutrons. The experimental facilities, some of which are unique, are used annually by more than 2,500 guest researchers from universities and other research organisations worldwide. Above all, HZB is known for the unique sample environments that can be created (high magnetic fields, low temperatures). HZB conducts materials research on themes that especially benefit from and are suited to large scale facilities. Research topics include magnetic materials and functional materials.
In the research focus area of solar energy, the development of thin film solar cells is a priority, whilst chemical fuels from sunlight are also a vital research theme. HZB has approx. 1,100 employees of whom some 800 work on the Lise-Meitner Campus in Wannsee and 300 on the Wilhelm-Conrad-Röntgen Campus in Adlershof.
HZB is a member of the Helmholtz Association of German Research Centres, the largest scientific organisation in Germany.