Thin-Film Solar Cells: New Insights into the Indium/Gallium Puzzle

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Scientists at Johannes Gutenberg University Mainz (JGU, Germany) have made a major breakthrough in their search for more efficient thin-film solar cells. Computer simulations designed to investigate the so-called indium/gallium puzzle have highlighted a new way of increasing the efficiency of CIGS thin-film solar cells. It has only proved possible to date to achieve an around 20% efficiency with CIGS cells although efficiency levels of 30% are theoretically possible. The work of the scientists in Mainz has been published in the latest edition of the leading journal *Physical Review Letters*.

Thin-film solar cells are gaining an ever increasing proportion of the solar cell market. As they are only a few micrometers thick, they offer savings on material and manufacturing costs. Currently, the highest level of efficiency of about 20% is achieved by CIGS thin-film solar cells, which absorb the sunlight through a thin layer made of copper, indium, gallium, selenium, and sulphur. However, the levels of efficiency achieved to date are nowhere near the levels theoretically possible.

The research team at Mainz University headed by Professor Dr Claudia Felser is using computer simulations to investigate the characteristics of CIGS, whose chemical formula is Cu(In,Ga)(Se,S)2. This research forms part of the comCIGS project funded by the Federal German Ministry for the Environment, Nature Conservation, and Nuclear Safety (BMU). IBM Mainz and Schott AG are collaborating with the Johannes Gutenberg University Mainz, the Helmholtz Center Berlin for Materials and Energy and Jena University in the project that is targeted at finding ways of optimizing CIGS solar cells. The researchers focused in particular on the indium/gallium puzzle that has been baffling scientists for years: Although it has been postulated on the basis of calculations that the optimal indium:gallium ratio should be 30:70, in practice, the maximum efficiency level has been achieved with the exactly inverse ratio of 70:30.

With the support of IBM Mainz, Christian Ludwig of Professor Felser's team undertook new calculations with the help of a hybrid method in which he used a combination of density functional calculations and Monte Carlo simulations. "Density functional calculations make it possible to assess the energies of local structures from the quantum mechanical point of view. The results can be used to determine temperature effects over wide length scale ranges with the help of Monte-Carlo simulations", Dr Thomas Gruhn, head of the theory group in Professor Felser's team, explains the methods used. Christian Ludwig is able to use a mainframe for his investigations that was recently donated to Mainz University by IBM as part of a Shared University Research (SUR) science award.

Production at high temperatures promotes homogeneity of the material

With the aid of the simulations, it was discovered that the indium and gallium atoms are not distributed evenly in the CIGS material. There is a phase that occurs at just below normal room temperature in which the indium and gallium are completely separate. If the material is heated to above this demixing temperature, differently sized clusters of indium and gallium atoms do form. The higher the temperature, the more homogeneous the material becomes. It has now become apparent that gallium-rich CIGS is always less homogeneous than indium-rich CIGS. Because of this lack of homogeneity, the optoelectronic properties of the gallium-rich material are poorer, resulting in the low efficiency levels of gallium-rich CIGS cells - an effect that has now been explained for the first time. The calculations also provide a concrete indication of the best way to manufacture CIGS solar cells. If it is produced at higher temperatures, the material is significantly more homogeneous. To retain the desired homogeneity, the material then needs to be cooled down sufficiently rapidly.

In practice, it was the limited heat resistance of the glass used as a substrate for solar cells that has always restricted process temperatures, but a significant breakthrough has also recently been made here. Schott AG has developed a special glass with which the process temperature can be increased to well above 600°C. The cells that result from this process are considerably more homogeneous, meaning that the production of cells with a much greater efficiency level has become possible. But the comCIGS project researchers are already thinking ahead of this. "We are currently working on large-format solar cells which should outperform conventional cells in terms of efficiency," states Gruhn. "The prospects look promising."

Provided by Johannes Gutenberg University Mainz