Forcing mismatched elements together could yield better solar cells

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(PhysOrg.com) -- In what could be a step toward higher efficiency solar cells, an international team including University of Michigan professors has invalidated the most commonly used model to explain the behavior of a unique class of materials called highly mismatched alloys.

Highly mismatched alloys, which are still in the experimental stages of development, are combinations of elements that won't naturally mix together using conventional crystal growth techniques. Professor Rachel Goldman compares them to some extent to homogenized milk, in which the high-fat cream and low-fat milk that would naturally separate are forced to mix together at high pressure.

New mixing methods such as "molecular beam epitaxy" are allowing researchers to combine disparate elements. The results, Goldman says, are more dramatic than smooth milk.

"Highly mismatched alloys have very unusual properties," Goldman said. "You can add just a sprinkle of one element and drastically change the electrical and optical properties of the alloy."

Goldman is a professor in the departments of Materials Science and Engineering, and Physics. Her team included other U-M physicists and engineers as well as researchers from Tyndall National Institute in Ireland.

Solar cells convert energy from the sun into electricity by absorbing light. However, different materials absorb light at different wavelengths. The most efficient solar cells are made of multiple materials that together can capture a greater portion of the electromagnetic radiation in sunlight. The best solar cells today are still missing a material that can make use of a portion of the sun's infrared light.

Goldman's team made samples of gallium arsenide nitride, a highly mismatched alloy that is spiked with nitrogen, which can tap into that underutilized infrared radiation.

The researchers used molecular beam epitaxy to coax the nitrogen to mix with their other elements. Molecular beam epitaxy involves vaporizing pure samples of the mismatched elements and combining them in a vacuum.

Next, the researchers measured the alloy's ability to convert heat into electricity. They wanted to determine whether its 10 parts per million of nitrogen were distributed as individual atoms or as clusters. They found that in some cases, the nitrogen atoms had grouped together, contrary to what the prevailing "band anti-crossing" model predicted.

"We've shown experimentally that the band anti-crossing model is too simple to explain the electronic properties of highly mismatched alloys," Goldman said. "It does not quantitatively explain several of their extraordinary optical and electronic properties. Atomic clusters have a significant impact on the electronic properties of alloy films."

If researchers can learn to control the formation of these clusters, they could build materials that are more efficient at converting light and heat into electricity, Goldman said.

"The availability of higher efficiency thermoelectrics would make it more practical to generate electricity from waste heat such as that produced in power plants and car engines," Goldman said.

More information: This research is newly published online in *Physical Review B*. The paper is entitled "Nitrogen composition dependence of electron effective mass in gallium arsenide nitride." Full text of paper: prb.aps.org/abstract/PRB/v82/i12/e125203

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