Using machine learning algorithms to understand solar cell degradation

There is new insight into what causes degradation effect of nanocrystalline solar cells which affects cell efficiency. Scientists use a genetic algorithm to analyze nanocrystalline structure data and predict what features are associated with degradation.

Amorphous silicon, along with nanocrystalline silicon, is a heavily researched material for photovoltaic applications. Its main benefit is that the cost of manufacturing is cheaper than crystalline solar cells and those cells can be grown on large areas. However, one of the main problems with these solar cells is that they experience performance degradation caused by exposure to light, called the Staeble Wronski effect which is not well understood. According to Dr. Tim Mueller, “The disordered nature of amorphous silicon is probably the main reason the Staebler-Wronski effect is poorly understood.” Dr. Tim Mueller, a professor at John Hopkins University, along with MIT Graduate student Eric Joshlin recently wrote a paper in which they use a genetic programming algorithm to link which structural features of nanocrystalline silicon are associated with hole traps, which contribute to the Staeble Wronski effect.

Studying the Staeble-Wroski effect is important because being able to accurately predict what causes degradation will allow us to optimize materials and create more efficient solar cells. In the paper, using a machine learning algorithm, Dr. Tim Mueller and Eric Joshlin predict that bridged bonds (Si-H-Si) play a direct role in the size of the whole traps and therefore are linked to the Staeble-Wronski effect. This prediction will help theorists that study amorphous thin films test new models.

Holes are quasi-particles that act as charge carriers in the valance band due to an absence of the corresponding electron. A hole trap is an area inside of a material, usually due to an imbalance of electrons, where the hole will recombine. It is thought that the size of the hole traps are linked to the light induced degradation. The size of the hole traps are measured by finding the difference in energy of a unit cell of the structure between when it is charged and neutral.

When removing an electron to measure the hole trap size, the Bravias lattice of the structure will and so approximation methods are used. “A simple way to think about this is that when you remove an electron from the unit cell, the electrostatic forces on the atoms will change. This will cause the atoms to shift a little bit, which causes the lattice vectors to shift a little bit. (In reality it's a bit more complicated than this.) “, explained Dr. Mueller. “I should

note that in a real amorphous material, there is no Bravais lattice. The Bravais lattice was introduced as an approximation for our calculations. Otherwise we would have to include a very large number of symmetrically distinct atoms in our calculations, which would take up a lot of computer time."

The task at hand was to calculate the hole depth of 1045 different nc-Si:H structures using computational tools. Each unit cell contained 216 silicon atoms and 20 hydrogen atoms. While computational analysis for amorphous silicon has been done it has only looked at a few features. This research examines how 242 material are associated with the largest hole traps. In order to find relationships between large data Dr. Mueller used a machine learning algorithm, a type of program that has the ability to learn and adjust itself based on input data. Specifically, he used a genetic programming algorithm which is: "a method of solving problems using computers through an analogue of natural selection. of a number of possible functions, the most effective functions survive and compete or cross-breed with other functions to continually approach closer to the needed solution." In this specific study, the functions contain variables that represent the 242 structural descriptors of the material.

On why he uses this type of algorithm, Dr. Mueller wrote: "I chose this method out of curiosity initially. It seemed like a good way to rapidly find patterns in the type of data set we had generated." He then explained the strengths and limitations of this anaylsis. "It works well in identifying descriptors because it is able to find non-linear relationships between combinations of descriptors and the hole trap depths. However it's a better method for identifying descriptors than it is for predicting hole trap depths."

The fitness of the function must be balanced by its complexity because simpler functions are more likely to over fit the data. The functions that have the closest balance between complexity and fitness are along a frontier plot (figure 3). The variables in these functions along the frontier are ones that are most likely to influence hole traps.. It was found that the features can be grouped as descriptors of three types of bonds: Bridge bonds, floating bonds and densely packed silicon.

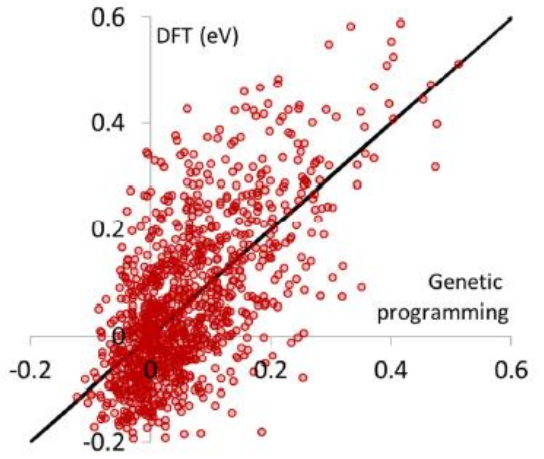

FIG. 3. (Color online) The DFT-calculated trap depths compared to those predicted by the function discovered by genetic programming. The black line indicates an ideal match.

Dr. Mueller explains the difference between floating bonds and dangling bonds: “A silicon atom with a dangling bond has only three nearest neighbors; a silicon atom with a floating bond has five. (Most silicon atoms have four nearest neighbors)”. Current theories predict that floating bonds are associated with hole traps while dangling bonds do not. From the analysis, descriptors that describe floating bonds are not the list of variables while descriptors for floating bonds are which shows that this analysis is consistent with prevailing theories.

Where this research gets interesting is that bridge bonds, a hydrogen atom bound to two silicon atoms, are significant contributors to hole densities. This was not something that was considered before and is also interesting because it shows hydrogen atoms play a role. The proposed theory is that when light hits the material, hydrogen is inserted into a weakened Si-Si bond, leaving behind a dangling bond. An increase in the bridge-bond concentration due to light soaking, as predicted by kinetic models, would likely result in the degradation of device performance.

This is something that will be explored further, however, Dr. Mueller currently has no plans to do further research “I'm not aware of any [further research], but I suspect there will be some. I'm not working on amorphous silicon any more, but if I were to get involved with it again I'd certainly consider exploring this result in more depth.”