

Experiment reveals that crystalline volume fraction is dependent on grain size for promising future thin-film photovoltaic material: nanocrystalline silicon

Nanocrystalline thin-film solar cells are generating interest for commercial use because they are not prone to light induced degradation. Researchers who are studying various properties of the thin-film have found that the volume fraction of the crystal has a dependence on crystallite size.

Thin-film solar cell technology has been a hot research area in condensed matter physics, especially since the sharp increase in gasoline prices in the mid-2000s. One promising material to use as the semiconductor material is nanocrystalline silicon, which has the benefit over standard amorphous silicon in that it has higher electron mobility, is not affected by degradation and has a higher absorption spectrum. Nanocrystalline silicon contains grains of silicon referred to as crystallites on the nano scale separated by amorphous silicon.

In order to understand how the grain size within the nanocrystalline silicon affects the volume concentration, Dr. Stephan O'Leary, Associate professor of the School of Engineering at University of British Columbia, along with graduate student Kathrin Schmidt, tested various nanocrystalline thin-film solar cell samples, each with different mean grain size. The results were published in the Canadian Journal of Physics on February 3rd 2014. They observed a statistically significant inverse relationship between the average crystallite size and overall crystalline volume fraction.

The main characteristic of an amorphous material is that it has no periodic order in its structure compared to a crystal. Bonds between atoms vary in strength. Some bonds will be completely broken leaving an unsatisfied valance known as a dangling bond. This results in an uneven charge distribution throughout the cell.

The advantage of using amorphous silicon for solar cells is that it is cheaper to manufacture and can be produced in large sizes compared to traditional monocrystalline wafer cells because it is grown onto a substrate. However, the main disadvantage (aside from lower efficiencies), according to Dr. O'Leary: "They experiences light induced degradation known as the Staebler-Wronski effect. This will reduce efficiency by up to 30% of a solar cell within a couple months of being exposed to the sun." Sunlight causes the density of defects to increase and this will increase the recombination rate. "The advantage of using nanocrystalline silicon thin film as solar cells is that, it tends to have more ordered and as a results the effect is minimized."

Nano crystalline silicon is similar to amorphous silicon in that it has no

long range order and a significant amount of defects. It is deposited onto a substrate using PECV deposition techniques. However, it has small crystal grains within the amorphous phase. Polycrystalline materials are similar, in that they have grains (in the micrometer scale) of crystal that have different orientations to one another separated by grain boundaries but they are not separated by an amorphous phase.

In their research, Dr. O'Leary and Schmidt set out to find if there is a relationship between the mean size of crystallite and the crystalline volume fraction. 11 different samples of nanocrystalline based thin film photovoltaic cells were observed. Each of these solar cells had the same structure: i.e. deposited on steel substrates, contain textured reflectors and the intrinsic layer has a 3 μm thickness. The main difference was the ratio of hydrogen that was diluted with the silane varied from 65 to 90.

In order to measure the average grain size, x-ray diffraction was used. The photovoltaic cells were sent to The Advanced Materials and Process Engineering Laboratory where Dr. Mario Beaudoin, research associate at AMPEL, was tasked to "perform the XRD scans and to discuss the XRD and Raman results". He observed peak intensity of silicon, [2 2 0] lattice plane, to be at 46 degrees. "There were peaks also peaks for silicon found at 28° [111] and 56° [3 1 1] for some samples but

were not used in the analysis because we wanted the results to be consistent for all cells." The Scherrer equation was then used to determine the mean crystallite size from the peak angles.

The Crystalline Volume Fraction was determined using Raman Spectroscopy by Dr. Guangrui Xia, member of the Microsystems and Nanotechnology research group at UBC. The excitation wavelength used is 442nm. The Raman Shift spectrum was decomposed into amorphous, grain boundary and crystalline components. The peak intensity of these components (occurring at 480 cm^{-1} , 510 cm^{-1} and 520 cm^{-1} shift respectively) was used to measure the crystalline volume fraction. The issue with the Raman Spectroscopy results was that the laser beam reduced in intensity by 10% by the p-doped layer by the time it reached the intrinsic layer which caused the Raman results to be influenced by the doped layer. This was because the penetration depth of the laser beam was 0.125 μm while the thickness of the p-doped layer is 15-20nm thick

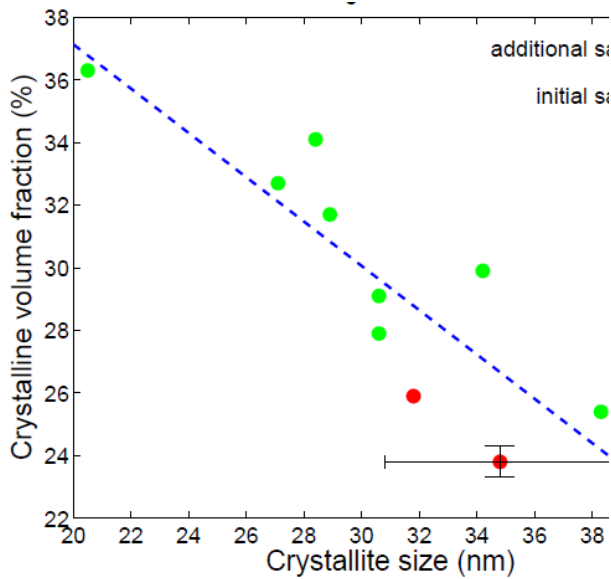


Figure 1: The crystalline volume fraction as a function of the mean crystallite size for the eleven nc-Si:H based photovoltaic solar cells considered in this analysis.

The data plotted (figure 1) shows that as the mean crystallite size of the solar cells increased the crystalline volume fraction decreased. Dr. O’Leary suggests the reason is that: “small crystallites can randomly pack with a greater packing fraction which would cause there to be a larger volume of crystalline.” However, this has not been confirmed by the experiment. Also, similar experiments have been performed by another research group in which they did there x-ray diffraction using [1 1 1] silicon peaks. In their analysis, crystalline volume fraction changed at a higher rate for similar crystallite sizes than in Dr. O’Leary’s experiment. Therefore, this dependency needs further analysis.