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The Materials Science of Chalcopyrite Materials for Solar Cell Applications

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This paper describes results for surface and bulk characterization of the most promising thin film solar cell material for high performance devices, (Ag,Cu) (In,Ga) Se2 (ACIGS). This material in particular exhibits a range of exotic behaviors. The surface and general materials science of the material also has direct implications for the operation of solar cells based upon it. Some of the techniques and results described will include scanning probe (AFM, STM, KPFM) measurements of epitaxial films of different surface orientations, photoelectron spectroscopy and inverse photoemission, Auger electron spectroscopy, and more. Bulk measurements are included as support for the surface measurements such as cathodoluminescence imaging around grain boundaries and showing surface recombination effects, and transmission electron microscopy to verify the surface growth behaviors to be equilibrium rather than kinetic phenomena. The results show that the polar close packed surface of CIGS is the lowest energy surface by far. This surface is expected to be reconstructed to eliminate the surface charge. However, the AgInSe2 compound has yielded excellent atomic-resolution images of the surface with no evidence of surface reconstruction. Similar imaging of CuInSe2 has proven more difficult and no atomic resolution images have been obtained, although current imaging tunneling spectroscopy images show electronic structure variations on the atomic scale. A discussion of the reasons why this may be the case is given. The surface composition and grain boundary compositions match the bulk chemistry exactly in as-grow films. However, the deposition of the heterojunction forming the device alters this chemistry, leading to a strongly n-type surface. This also directly explains unpinning of the Fermi level and the operation of the resulting devices when heterojunctions are formed with the CIGS. These results are linked to device performance through simulation of the characteristic operating behaviors of the cells using models developed in my laboratory.