

SYNTHESIS AND CHARACTERIZATION OF Cu_2Se NANOPARTICLES FOR PHOTOVOLTAIC APPLICATIONS: AEROBIC SURFACE OXIDATION

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Copper selenide thin films and nanoparticles have received increasing attention with their potential applications in high efficiency solar cells^{1,2}, photovoltaic devices³, as well as numerous other applications. The wide array of possible electric and optoelectric applications for copper selenide stem from the plethora of stoichiometric (CuSe , Cu_2Se , Cu_3Se_2 , CuSe_2) and nonstoichiometric (Cu_{2-x}Se) compositions; thereby leading to variations in the crystal structure, band gap energies, and oxidation state of the Cu and Se.

Copper (I) selenide is a p-type semiconductor with a widely varying indirect band gap of 1.1-1.5 eV and a direct band gap of 2.0-2.3 eV⁴. The indirect band gap lies near the optimal value for solar cell applications when exhibiting semiconductor behavior. Some researchers, however, report ohmic type behavior, which, in turn, can hinder the efficiency of the solar cell. We have, therefore, synthesized Cu_2Se nanoparticles and tracked its stability through X-ray photoelectron spectroscopy and X-ray diffraction studies, as well as monitored the electronic properties of a nanoparticle thin film as a function of air exposure through current-voltage measurements. Upon exposing the nanoparticles to air, gradual oxidation of Cu^{+1} and Se^{-2} occurs immediately, ultimately leading to a change in crystal structure. The electronic properties of Cu_2Se nanoparticle thin film parallel the observed oxidation and change in crystal structure. As illustrated in Figure 1, Cu_2Se exhibits semiconducting behavior under an inert atmosphere. However, as the stoichiometry and crystal structure evolve as a result of oxygen exposure, the semiconductor response is quickly converted to an ohmic one within hours of air exposure.

The current focus is the design and characterization—through current density-voltage and photocurrent studies—of a Cu_2Se nanoparticle thin film heterojunction solar cell. During that process, spectrophotometer measurements of the unoxidized particles will also be conducted to confirm the indirect and direct band gap energies. These measurements are crucial, as there is

some discrepancy in the literature regarding the direct band gap, which can possibly be attributed to the formation of a surface copper oxide.

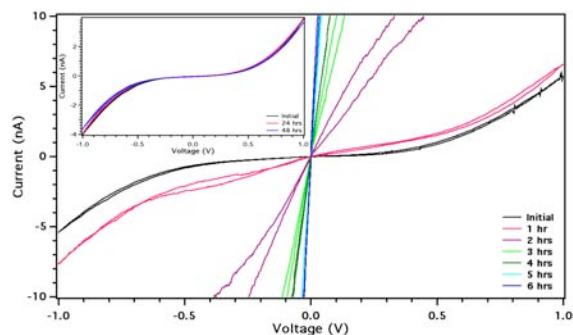


Figure 1. Current-voltage measurements taken as a function of air exposure over a 6-hour period. The inset shows the semiconducting behavior of the film for initial, 24 hour, and 48 hour I-V measurements taken inside a nitrogen glove box.

1. Chen, W. S.; Stewart, J. M.; Mickelsen, R. A. *Applied Physics Letters* **1985**, 46, (11), 1095-1097.
2. Okimura, H.; Matsumae, T.; Makabe, R. *Thin Solid Films* **1980**, 71, (1), 53-59.
3. Mane, R. S.; Kajve, S. P.; Lokhande, C. D.; Han, S. H. *Vacuum* **2006**, 80, (6), 631-635.
4. Pathan, H. M.; Lokhande, C. D.; Amalnerkar, D. P.; Seth, T. *Applied Surface Science* **2003**, 211, (1-4), 48-56.