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Origin of reduced efficiency in high Ga concentration $Cu(In,Ga)Se_2$ solar cell S.-H. WEI, B. HUANG, H. DENG, M.A. CONTRERAS, R. NOUFI, National Renewable Energy Laboratory, S. CHEN, L.W. WANG, Lawrence Berkeley National Laboratory — $CuInSe_2$ (CIS) is one of the most attractive thin-film materials for solar cells. It is well know that alloying Ga into CIS forming $Cu(In,Ga)Se_2$ (CIGS) alloy is crucial to achieve the high efficiency, but adding too much Ga will lead to a decline of the solar cell efficiency. The exact origin of this puzzling phenomenon is currently still under debate. Using first-principles method, we have systemically studied the structural and electronic properties of CIGS alloys. Our phase diagram calculations suggest that increasing growth temperature may not be a critical factor in enhancing the cell performance of CIGS under equilibrium growth condition. On the other hand, our defect calculations identify that high concentration of antisite defects M_{Cu}(M=In, Ga) rather than anion defects are the key deep-trap centers in CIGS. The more the Ga concentration in CIGS, the more harmful the deep-trap is. Self-compensation in CIGS, which forms $2V_{Cu}+M_{Cu}$defect complexes, is found to be beneficial to quench the deep-trap levels induced by M_{Cu} in CIGS, especially at low Ga concentration. Unfortunately, the density of isolated M_{Cu} is quite high and cannot be largely converted into $2V_{Cu}+M_{Cu}$ complexes under thermal equilibrium condition. Thus, nonequilibrium growth conditions or low growth temperature that can suppress the formation of the deep-trap centers M_{Cu} may be necessary for improving the efficiency of CIGS solar cells with high Ga concentrations.

Suhuai Wei
NREL

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