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Theoretical study on the growth conditions for single-phase stability of kesterite-Cu_2ZnSnS_4[1] PRANAB SARKER, TYLER J. HARRISON, Department of Physics, University of Texas at Arlignton, MOWAFAK M. AL-JASSIM, Analytical Microscopy, National Renewable Energy Laboratory, MUHAMMAD N. HUDA, Department of Physics, University of Texas at Arlignton — Nowadays, kesterite-Cu_2ZnSnS_4 (CZTS) is being pursued as an efficient solar absorber materials for PV cells. By chemical potential landscape analysis of CZTS we will show that the formation of stoichiometric CZTS is practically impossible at thermodynamic equilibrium. This analysis verifies the experimental fact that non-stoichiometry is evident for high efficiency CZTS. In addition, the co-existence of ZnS is found to be highly probable if high efficiency growth condition (Zn rich, Cu-poor) is pursued. Moreover, it is found that Zn-richer growth condition is necessary to minimize the number of competitive secondary phases. Cu-poor condition should be chosen in such a way so that the occurrence of Cu_2S can be prevented irrespective of the value available chemical potential for S. In addition, defect calculation shows that the suitable Cu-poor condition can prevent anionic defects as well.

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