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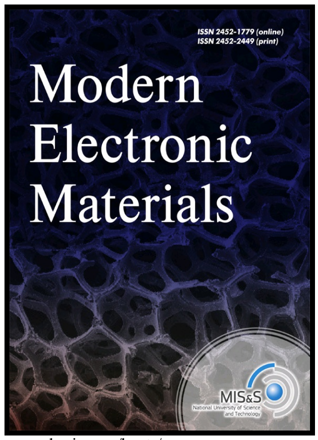

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Study of optimization options for second generation solar cell materials by multilevel modeling

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Abstract

Theoretical analysis of optimization options for the properties of CdTe absorber layer is an important task for increasing the efficiency of CdTe/CdS heterojunction based thin-film solar cells. Properties of the materials (e.g. the density of free carriers) often depend essentially on the parameters of the deposition process and subsequent treatment which determine the defect composition of the material. In this work a model based on the lattice kinetic Monte-Carlo method is developed to describe the process of CdTe deposition as a function of temperature and Cd and Te fluxes. To determine the effect of the treatment conditions on CdTe conductivity, we developed a quasichemical model based on the electrical neutrality equation for point defect concentrations that are described by defect formation reaction constants. Parameters obtained from the first-principles density functional calculations were used for developing the models. The developed deposition model correctly describes the transition from evaporation to precipitation as well as the increased evaporation rates in excess of Cd. To explain the observed electrical properties of CdTe after Cl-treatment, we complemented the quasichemical defect model by a deep acceptor complex defect that allowed us to describe both the high-temperature dependence of conductivity on the Cd pressure and the dependence of resistivity on Cl concentration at room temperature.

Keywords

Multi-scale modeling, kinetic Monte Carlo, first principles calculations, quasichemical model for point defects, II-VI semiconductors, defects in crystals, solar cells

Introduction

Thin film solar cells based on CdTe/CdS heterojunction have reached a lab efficiency of 19.6% which is comparable with the competing technologies based on silicon thin films in CuInGaSe [1]. There is however a significant gap between the efficiency of even the best lab specimens and the theoretical