Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Mechanisms and Kinetics of Tellurium Precipitation in CdTe-based Materials VINCENZO LORDI, Lawrence Livermore National Lab — CdTe and related alloys are important materials for solar photovoltaic application as well as for high-resolution room-temperature gamma radiation detectors. However, the performance of devices, particularly in high-energy applications, is limited by various material defects. Among the most important defects are Te precipitates of various sizes caused by non-stoichiometric growth conditions. In this work, we study the kinetics of Te aggregation and precipitation at the atomic scale. Density functional theory is used to compute the energetics, migration rates, and binding energies of point defects involved in Te aggregation, which include various interstitials, vacancies, and anti-site defects. Kinetic Monte Carlo is then used to simulate the aggregation process leading to precipitation nuclei. The mechanisms and kinetics of formation of these Te-rich regions are analyzed for various conditions. Prepared by LLNL under Contract DE-AC52-07NA27344.

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Date submitted: 10 Nov 2011 Electronic form version 1.4