MAR13-2012-008268

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Point Defect Properties of Cd(Zn)Te and TlBr for Room-Temperature Gamma Radiation Detectors[1]

VINCENZO LORDI, Lawrence Livermore National Laboratory

The effects of various crystal defects in CdTe, $Cd_{1-x}Zn_xTe$ (CZT), and TlBr are critical for their performance as room-temperature gamma radiation detectors. We use predictive first principles theoretical methods to provide fundamental, atomic scale understanding of the defect properties of these materials to enable design of optimal growth and processing conditions, such as doping, annealing, and stoichiometry. Several recent cases will be reviewed, including (i) accurate calculations of the thermodynamic and electronic properties of native point defects and point defect complexes in CdTe and CZT; (ii) the effects of Zn alloying on the native point defect properties of CZT; (iii) point defect diffusion and binding related to Te clustering in Cd(Zn)Te; (iv) the profound effect of native point defects—principally vacancies—on the intrinsic material properties of TlBr, particularly electronic and ionic conductivity; (v) tailored doping of TlBr to independently control the electronic and ionic conductivity; and (vi) the effects of metal impurities on the electronic properties and device performance of TlBr detectors.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344 with support from the National Nuclear Security Administration Office of Nonproliferation and Verification Research and Development NA-22.