Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Theoretical study of the deep defect states in PbTe thin films[1]
KHANG HOANG, S.D. MAHANTI, Michigan State University, P. JENA, Virginia Commonwealth University — The nature of deep defect states (DDS) in bulk PbTe has been studied recently using density functional theory and a supercell model [1]. It was found that substitution of Pb by the trivalent impurities Ga, In, and Tl gave rise to hyperdeep defect states (HDS) below the valence band (VB) and DDS near the band gap region. Here we discuss how these states are affected in a (100) PbTe film using a supercell slab model. The HDS and DDS are preserved in the film geometry. As one goes from the bulk-like layers to subsurface and surface layers, the HDS tends to move closer to the bottom of the VB and becomes narrower; the DDS also gets modified. We also find that the defect formation energy E_f as a function of the distance from the surface shows interesting features: all three impurities have lowest E_f in the first layer but E_f increases monotonically in the case of Ga, whereas there is a potential barrier in the second layer and a shallow potential "valley" between the second and the bulk-like layers in the case of In and Tl. This suggests that Ga impurities will be annealed out whereas the other two can be trapped in the subsurface region. [1] Salameh Ahmad, Khang Hoang, and S. D. Mahanti, Phys. Rev. Lett. 96, 056403 (2006).

[1]Work in VCU partially supported by DOE.

Khang Hoang
Michigan State University

Date submitted: 21 Nov 2006 Electronic form version 1.4