Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Kinetic barriers for Cd and Te adatoms on Cd and Te terminated CdTe (111) surface using *ab initio* **simulations**[1] EBADOLLAH NADERI, Department of Physics, University of Pune, Pune 411007, SACHIN P. NANAVATI, C-DAC, Pune University, Pune 411007, India, CHIRANJIB MAJUMDER, Bhabha Atomic Research Center, Mumbai 400085, India, S.V. GHAISAS, Department of Electronic Science, University of Pune, Pune 411007 — In the present work we have calculated using density functional theory (DFT), diffusion barrier potentials on both the CdTe (111) surfaces, Cd terminated (A-type) & Te terminated (B-type). We employ nudge elastic band method (NEB) for obtaining the barrier potentials. The barrier is computed for Cd and for Te adatoms on both A-type and B-type surfaces. We report two energetically favourable positions along the normal to the surface, one above and other below the surface. The one above the surface has binding energy slightly more the one below. According to the results of this work, binding energy (in all cases) for adatoms are reasonable and close to experimental data. The barrier potential for hopping adatoms (Cd and Te) on both the surfaces is less than 0.35 eV. Apart from these most probable sites, there are other at least two sites on both the types of surfaces which are meta stable. We have also computed barriers for hopping to and from these meta stable positions. The present results can shade light on the defect formation mechanism in CdTe thin films during growth.

[1]The authors would like to thank C-DAC for the computing time on its PARAM series of supercomputers and DST Govt. of India, for partial funding.

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Date submitted: 15 Nov 2013 Electronic form version 1.4