

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Diffusion of a Ga adatom on the GaAs(001)- $c(4 \times 4)$ -heterodimer surface: A first-principles study¹ SANJAY KHARE, JASON ROEHL, SANDEEP ARAVELLI, University of Toledo, RAY PHANEUF, University of Maryland — The adsorption and diffusion behavior of a Ga adatom on the GaAs(001)- $c(4 \times 4)$ -heterodimer surface were studied by employing ab initio density functional theory computations in the local density approximation. Structural and bonding features of the $c(4 \times 4)$ -heterodimer reconstruction surface were examined. A comparison with the $c(4 \times 4)$ -ss reconstruction² was performed. Minimum energy sites (MES) on $c(4 \times 4)$ -heterodimer surface were located by mapping the potential energy surface for a Ga adatom. Barriers for diffusion of a Ga adatom between the neighboring MES were calculated by using top and exchange diffusion mechanisms. We proposed two unique diffusion pathways for a Ga adatom diffusing between the global minimums of two neighboring unit cells. Signature differences between electronic structures of top- and exchange- diffusion mechanisms were studied for relevant atoms. We observed a higher diffusion barrier for exchange mechanism compared to top hopping.³

¹Submitted for publication.

²J. L. Roehl et al, Phys. Rev. B 82, 165335 (2010).

³Supported by NSF DMR 0705464, CNS 0855134.

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Date submitted: 13 Nov 2011

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