Surface Science 606 (2012) 1303–1307

Contents lists available at SciVerse ScienceDirect

Surface Science

journal homepage: www.elsevier.com/locate/susc

Diffusion of a Ga adatom on the GaAs(001)-$c(4\times4)$-heterodimer surface: A first principles study

J.L. Roehl [a], S. Aravelli [b], S.V. Khare [a,*], R.J. Phaneuf [c]

[a] Department of Physics and Astronomy, The University of Toledo, 2801 West Bancroft Street, Toledo, OH 43606, United States
[b] Department of Electrical Engineering and Computer Science, The University of Toledo, 2801 West Bancroft Street, Toledo, OH 43606, United States
[c] Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, United States

ARTICLE INFO

Article history:
Received 30 September 2011
Accepted 11 April 2012
Available online 24 April 2012

Keywords:
Gallium arsenide (001) surface
Adsorption
Diffusion barriers
Reconstruction
Density functional calculations

ABSTRACT

The adsorption and diffusion behavior of a Ga adatom on the GaAs (001)-$c(4\times4)$-heterodimer surface were studied by employing *ab initio* density functional theory (DFT) computations in the local density approximation. Structural and bonding features of the $c(4\times4)$-heterodimer reconstruction surface were examined. A comparison with the $c(4\times4)$-ss reconstruction was performed. Minimum energy sites (MES) on the $c(4\times4)$-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 hopping- 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 hopping- and exchange-diffusion mechanisms were studied for relevant atoms. We observed a higher diffusion barrier for exchange mechanism compared to top hopping.

© 2012 Elsevier B.V. All rights reserved.

1. Introduction

Gallium arsenide (GaAs), a III–V group semiconductor, has useful electronic and optical properties. Several applications from solar cells, to light emitting diodes and other optoelectronic devices, make GaAs a well studied material [1]. The GaAs(001) surface is the one of the most frequently studied surfaces during growth by molecular beam epitaxy (MBE). A great deal of work has been done, both theoretically and experimentally, to provide in depth understanding into MBE growth on GaAs(001) [2]. This work has included surface morphology, step-flow layer growth and island nucleation using a number of experimental techniques, such as reflection high-energy electron-diffraction (RHEED) intensity oscillations and scanning tunneling microscopy (STM) measurements, and theoretical modeling including kinetic Monte Carlo (KMC) simulations. The template for growth is normally produced by growing a so-called buffer layer by MBE for which the equilibrium surface reconstruction is generally accepted to be the β_2 (2×4) structure [2]. This has led to extensive work studying the behavior of Ga adatoms on the β_2 (2×4) surface reconstruction [3,4]. This work included mapping the β_2 (2×4) potential energy surface and MES and computing energy barriers required for diffusion between neighboring MES [3]. Subsequent work on the β_2 (2×4) surface, using a new semi-empirical potential for GaAs, included investigation of subsequent surface properties related to diffusion [4]. Our work differs from those in Refs. [3,4] in two ways. (i) Both papers focus on the β_2 (2×4) reconstruction of the GaAs(001) surface while our work is on the $c(4\times4)$-heterodimer surface. (ii) A second distinction comes from the methods used. Ref. [3] applies DFT based methods and a grid of the potential energy surface (PES) based on computations of MES on the β_2 (2×4) surface while we used the nudged elastic band (NEB) method on the $c(4\times4)$-heterodimer surface. Computations in Ref. [4] are based on semi-empirical potentials unlike our DFT based methods. There is no DFT work on diffusion barriers for a Ga adatom diffusing on the $c(4\times4)$-heterodimer surface that is the focus of the present study.

Dimerization of surface atoms is a common theme observed in several tetrahedrally coordinated semiconductor surfaces [3,5,6]. The GaAs(001) surface is no exception, with the As-rich $c(4\times4)$-ss reconstruction observed as the dominant surface during low temperature molecular beam epitaxial growth. This structural model with three As_2 dimers per surface unit cell was established by Sauvage-Simkin et al. [7] using grazing incidence X-ray diffraction and it was found to be stable at As-rich conditions by first principles calculations [8–11]. Recently Ohtake et al. [12] proposed a new structure model for $c(4\times4)$ reconstruction with three Ga–As heterodimers per unit cell. They proposed this model based on rocking-curve analysis of RHEED, STM, and reflectance difference spectroscopy. This new heterodimer (hd) structure was found to be consistent with element specific X-ray diffraction [13]. This structure referred to henceforth as the GaAs(001)-$c(4\times4)$-hd reconstruction consists of alternating rows of three Ga–As heterodimers followed by a missing dimer. The binding energies and diffusion barriers for a Ga adatom are unknown for this recently discovered GaAs(001)-$c(4\times4)$-hd surface reconstruction.

* Corresponding author. Tel.: +1 419 530 2292.
E-mail address: sanjay.khare@utoledo.edu (S.V. Khare).

0039-6028/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2012.04.014

We present results of first principles calculations on the GaAs (001)-$c(4\times4)$-hd surface reconstruction using DFT. Some structural differences between GaAs (001)-$c(4\times4)$-ss and GaAs(001)-$c(4\times4)$-hd reconstructions are highlighted. In particular, we report the energetics of Ga adatom diffusion on this reconstruction by top hopping and exchange mechanisms. From these results we propose different diffusion pathways for Ga adatom mass transport. Electronic structure differences in these different diffusion modes are investigated.

2. Computational method

The Vienna *ab initio* simulation package (VASP) [14–17] of codes was used to perform our first principles total energy calculations within the local density approximation (LDA) to DFT [18]. LDA yields good relative bond energies for highly coordinated atoms (e.g. surface energies and diffusion barriers on surfaces) [19]. The Ceperly–Alder exchange-correlation functional was used along with the ultrasoft-Vanderbilt type pseudo potentials [20] as supplied by Kresse et al. [21]. For each calculation, k points were generated according to the Monkhorst–Pack scheme [22] with a density equivalent to 32 k points in the Brillouin zone of the (1×1) surface cell. The energy cutoff used in expanding the single-particle wave functions was 150 eV. Tests using a higher plane-wave energy cutoff (250 eV) indicated that a numerical convergence better than ±5 meV was achieved, tests using a larger k-point sampling (64 instead of 32 k points) indicated that a numerical convergence better than ±2 meV was achieved. The minimum energy for each configuration was obtained by fully relaxing all atoms until a force convergence to less than 0.01 eV/Å was achieved. Based on this we estimated the error in the difference between total energies of different structures to be on the order of ±10 meV. Identical parameters were used to compute binding energies and diffusion barriers on the GaAs (001)-$c(4\times4)$-ss surface reconstruction [23]. For a Ga adatom relaxing from 3 Å in the trenches, LePage et al. [11] obtained results comparable with the results on the $c(4\times4)$-ss surface reconstruction [23]. Slight differences in numerical values may be attributed to variations in our methods (e.g. LePage's supercell was of half the area of our supercell). The value of the lattice constant was found to be 5.60 Å for the absolute minimum in total energy. It was within 0.9% of the experimental value of 5.65 Å [24]. The Methfessel–Paxton scheme [25] was used to calculate the local density of states (LDOS).

The diffusion barriers for the Ga adatom between two minimum energy sites (MES) on the surface were calculated using the nudged elastic band (NEB) method [26]. The NEB method works by performing collective minimizations of a number of linearly interpolated images of the Ga adatom between two MES. The configuration of the surface with the Ga adatom corresponding to the highest energy, along the diffusing path, is taken to be the transition point. The difference in energy between this transition point and initial MES is taken as the diffusion barrier. Diffusion barriers via the exchange mechanism between two MES involve a Ga adatom and a Ga atom in the heterodimer. The Ga atom in the heterodimer is displaced by the Ga adatom diffusing from an initial MES resulting in the Ga atom of the heterodimer moving to the final MES.

3. Modeling approach

Modeling the GaAs (001)-$c(4\times4)$-hd reconstruction was performed by constructing a six layer slab cut out of bulk GaAs. Each square layer was cut along the [1, 1, 0] and [−1, 1, 0] directions and contained 16 atoms. The Ga–As heterodimers on the slab surface, with [0, 0, 1] surface normal, were constructed by adding additional Ga and As adatoms to the top As bulk layer. The dangling bonds of the Ga layer on the bottom of the slab were passivated with a layer of hydrogen atoms. The hydrogen atoms were allowed to relax completely. We determined from vacuum tests on the slab that a vacuum layer thickness of 12 Å was required to eliminate the interactions between super cells. The vacuum layer and the slab had a combined height of 26.17 Å. The final reconstructed $c(4\times4)$-hd surface was obtained by relaxing the top 4 layers of the slab. Our final reconstructed surface was compared to that of Ohtake et al. [12] and found to be in excellent agreement. Measurements of surface atom displacements from their bulk positions were compared between our surface and that of Ohtake and the small average difference of 0.04 Å per degree of freedom can be attributed to the differences in our computed bulk GaAs bond length of 2.43 Å and Ohtake's computed bulk length of 2.45 Å. Such differences are expected from variations in the implementation of DFT methods.

The MES on the $c(4\times4)$-hd surface were calculated at sites obtained from the potential energy surface (PES) of a Ga adatom mapped over the irreducible part of $c(4\times4)$-hd surface. We mapped the PES by constructing a square 1 Å × 1 Å uniform grid above the surface. A Ga adatom was placed at each (X, Y) point on the grid at a distance of 3 Å above the reference surface height. The reference surface height was calculated by averaging the Z-coordinates of all neighboring surface atoms. The Ga adatom was constrained in the X and Y directions and allowed to relax unconstrained along the Z direction until the forces converged. The top four layers of the slab were allowed to relax for all the force convergence runs. The PES was interpolated from the relaxed energies computed at these grid points. A smaller grid, with a spacing of 0.2 Å × 0.2 Å, was constructed above low energy areas identified on the PES to determine potential MES. Final MES were obtained by allowing the Ga adatom to relax unconstrained above the potential MES points. The diffusion barriers between nearest neighbor MES were calculated by using NEB method.

4. Results and discussion

Structural differences between the GaAs (001)-$c(4\times4)$-ss [23] and GaAs(001)-$c(4\times4)$-hd reconstructions are shown in Fig. 1. A noticeable difference between the two reconstructions is the angle the dimers (heterodimers) make with the [0, 0, 1] surface normal. The Ga atoms in Ga–As heterodimers of the $c(4\times4)$-hd reconstruction are nearly incorporated completely into the surface resulting in

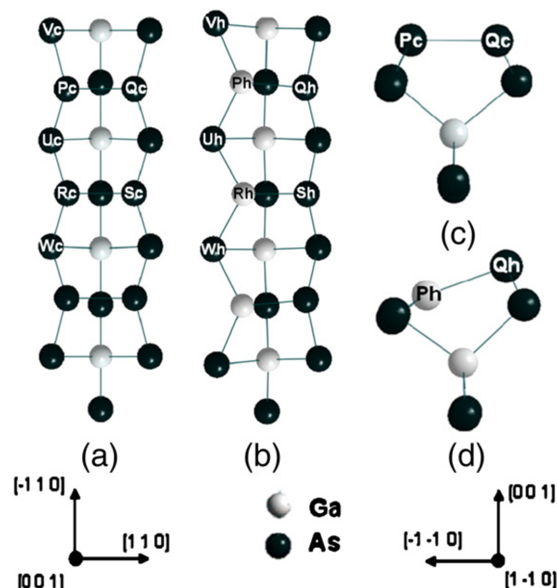

Fig. 1. Top view of rows of As_2 dimers on (a) GaAs (001)-$c(4\times4)$-ss and Ga–As dimers on (b) GaAs (001)-$c(4\times4)$-hd reconstruction. Side views of the $c(4\times4)$-ss and $c(4\times4)$-hd reconstructions are shown in (c) and (d) respectively to illustrate the heterodimer tilt. The As_2 dimers on the $c(4\times4)$-ss surface reconstruction are parallel to each other and lie perpendicular to the surface normal. The Ga–As dimers on $c(4\times4)$-hd surface tilt away from the mid-dimer with the Ga atoms moving farther apart. Quantitative structural differences between the reconstructions are given in Table 1.

Table 1
Structural diffreneces between GaAs (001)-$c(4\times4)$-ss and GaAs (001)-$c(4\times4)$-hd surfaces are shown. Atom labels are referred from Fig. 1. The last two rows give the angle between the surface normal and the surface dimers.

Parameter	$c(4\times4)$-ss	$c(4\times4)$-hd
$\lvert\overrightarrow{PQ}\rvert$	2.56 Å	2.47 Å
$\lvert\overrightarrow{RS}\rvert$	2.53 Å	2.43 Å
$\angle$VPU	110.4°	122.8°
$\angle$VPQ	103.5°	120.7°
$\angle$UPQ	103.9°	115.2°
$\angle$URW	103.3°	114.3°
$\angle$URS	104.2°	121.8°
$\angle$WRS	104.2°	121.8°
[0, 0, 1] ^ (edge dimers)	90°	106.5°
[0, 0, 1] ^ (mid dimer)	90°	104.6°

an extreme tilt of the heterodimers. The middle and edge Ga–As heterodimers lie at an angle of 106.5° and 104.6° to the [0, 0, 1] surface normal respectively, whereas the As_2 middle and edge dimers on $c(4\times4)$-ss reconstruction are perpendicular to the normal. The angle between the bonds formed by the Ga atom, labeled Ph and the two As sub surface atoms, labeled Vh and Uh is 122.8°. The angle between the bonds formed by the same Ga atom with the As sub surface atom, Vh and the As heterodimer atom, Qh is 120.7°. The angle between the bonds formed by the same Ga atom with the As sub surface atom, Uh and the As heterodimer atom, Qh is 115.2°. The average of these three angles is 119.5°. This is reminiscent of graphite like planar bonding with sp^2 hybridized electronic bonds, with bond angles of 120° each [27]. This contrasts with the $c(4\times4)$-ss case, where an As atom replaces the Ga atom and the corresponding angles are 110.4°, 103.5° and 103.9° respectively. The average of these angles is 105.9°. This is closer to the ideal value (109.5°) for sp^3 hybridized bonded bulk GaAs structure. Similar angles for both reconstructions at Ga, As atoms of mid-dimers, labeled Rh and Rc are given in Table 1. Also calculated on the $c(4\times4)$-hd reconstruction is a reduction in the bond lengths of edge (PQ) and middle (RS) dimers of 3.5% and 3.9% respectively, compared to those in the $c(4\times4)$-ss reconstruction. These quantitative differences are summarized in Table 1.

The MES for a Ga adatom on the $c(4\times4)$-hd reconstruction are shown in Fig. 2. We obtained a binding energy of 2.95 eV for the global minimum energy site C2. The binding energies of all MES are shown in Table 2. The presence of heterodimers on the surface forms hills along

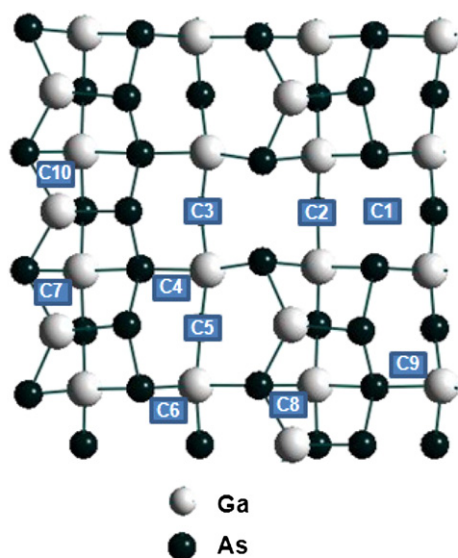

Fig. 2. Minimum energy sites (MES), labeled Cn where n varies from 1 to 10, obtained by relaxing a Ga adatom from 3 Å above the GaAs (001)-$c(4\times4)$-hd surface reconstruction.

Table 2
Binding energies of Ga adatom relaxed from 3 Å above the GaAs(001)-$c(4\times4)$-hd surface. The binding energies are given relative to the global minimum energy site C2 which has a binding energy of 2.95 eV.

Site	Energy (eV)
C1	0.24
C2	0
C3	0.37
C4 (C9)	0.61
C5	0.63
C6	0.56
C7 (C8, C10)	0.78

[−1, 1, 0] direction. The surface region between these hills is referred to as the trench. The C7 site, and equivalent C8 and C10 are located between the Ga–As heterodimers, on the hill. And all other MES appear in the trench region. Our computed structures show differences between the MES pattern of $c(4\times4)$-hd reconstruction compared to the $c(4\times4)$-ss reconstruction [23]. Four different MES are present in trench along the [−1, 1, 0] direction on the $c(4\times4)$-hd reconstruction compared to only two different MES along the same direction on the $c(4\times4)$-ss reconstruction. Furthermore, the three MES present in trench along the [1, 1, 0] direction on the $c(4\times4)$-hd reconstruction have different energies. In contrast, two of the three MES along the same direction on the $c(4\times4)$-ss reconstruction have the same energy. This difference can be explained by considering the symmetry of the two surface reconstructions. The $c(4\times4)$-ss surface reconstruction contains a mirror plane that bisects the As_2 dimer bonds along the [−1, 1, 0] direction. This mirror plane passes through the global minimum site so the MES on either side of this site have the same energy. The $c(4\times4)$-hd reconstruction does not possess this symmetry. The symmetry is broken by the presence of the Ga–As heterodimer. As a result, the MES labeled C1 and C3, on either side of the global minimum C2, face different types of atoms. MES C1 and C3 are now adjacent to Ga and As atoms respectively from the neighboring rows of heterodimers.

Diffusion barriers were calculated using the NEB method, as explained in Section 2. These barriers for both regular and the exchange mechanism are given in Table 3. The differences in diffusion barriers

Table 3
Diffusion barriers for Ga adatom on GaAs(001)-$c(4\times4)$-hd surface. Diffusion barriers for exchange mechanism are labeled with an E.

Diffusion pathway	Diffusion barrier (eV)
C1–C2	0.04
C2–C1	0.28
C2–C3	0.42
C3–C2	0.06
C3–C4	0.30
C4–C3	0.06
C4–C5	0.05
C5–C4	0.02
C5–C6	0.02
C6–C5	0.09
C6–C1	0.12
C1–C6	0.45
C1–C8	0.76
C1–C8-E	1.19
C8–C1	0.21
C8–C1-E	0.64
C5–C8	0.51
C5–C8-E	0.80
C8–C5	0.36
C8–C5-E	0.65
C7–C10 (C10–C7)	0.35
C8–C9	0.21
C9–C8	0.37
C8–C2	0.43
C8–C2-E	0.81
C2–C8	1.21
C2–C8-E	1.60

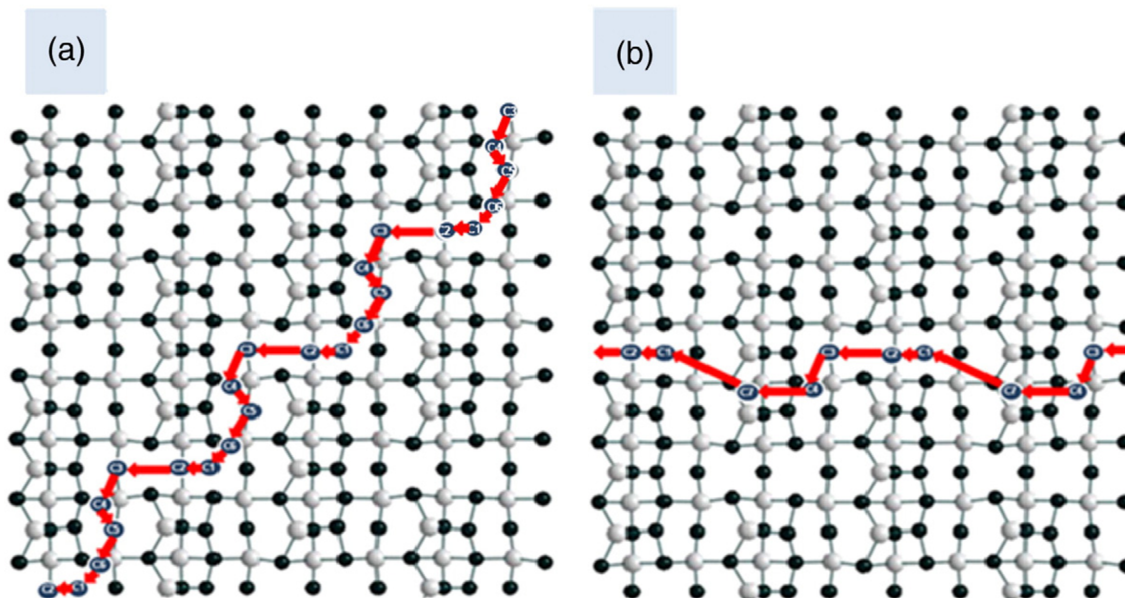

Fig. 3. Two non-collinear diffusion paths of a Ga adatom on the GaAs (001)-$c(4\times4)$-hd surface. Path (a) occurs between MES C2–C3–C4–C5–C6–C1–C2. The limiting step in this path is the 0.42 eV barrier between C2 and C3 along the [0–1 0] direction and 0.45 eV between C1 and C6 along [0 1 0]. Path (b) occurs between MES C2–C3–C4–C8–C1–C2. The limiting step in this path is the 0.42 eV barrier between C2 and C3 along the [−1 −1 0] direction and 0.76 eV between C1 and C8 along [1 1 0].

between neighboring MES (e.g. C1–C2 does not equal C2–C1) is explained by considering the relative binding energies of the initial and final MES, given in Table 2. The difference in energy between the transition point and initial MES is taken as the diffusion barrier for the first path, the difference in energy between the transition point and final MES represents the diffusion barrier for the return path. From the computed diffusion barriers we propose two non-collinear diffusion paths, shown in Fig. 3, for a Ga adatom diffusing from the global minimum (C2) to another C2 site in a neighboring unit cell. The first path, (a), shown in Fig. 3 occurs only by hops from MES in the trench. For diffusion along the [0–1 0] direction, this occurs between MES C2–C3–C4–C5–C6–C1–C2. For diffusion in the opposite direction, along the [0 1 0] direction, this occurs in the reverse order. The limiting step in the forward path is the 0.42 eV barrier between C2 and C3 along the [0–1 0] direction and 0.45 eV between C1 and C6 along [0 1 0]. The second diffusing path, (b), occurs both in the trench and over the dimer rows. For diffusion along the [−1 −1 0] direction this occurs between MES C2–C3–C4–C8–C1–C2, for diffusion along [1 1 0], the MES order is reversed. The limiting steps in these paths are the 0.42 eV barrier between C2 and C3 along [−1 −1 0] and 0.76 eV between C1 and C8 along [1 1 0]. We report a higher diffusion barrier for the exchange mechanism compared to the regular, top hopping mechanism between MES. This difference may be explained by the bonding configuration of the Ga heterodimer atom involved in the exchange mechanism. The Ga atom in the heterodimer, shown in Fig. 4(a), bonds with the two As subsurface atoms and the As heterodimer atom. The resulting configuration is close to being planar, similar to that in sp^2 hybridization. The additional energy required for the exchange mechanism, may be explained as the additional energy required by the incoming Ga adatom to break the favorable sp^2 like bonding configuration before replacing the Ga heterodimer atom. We explored this feature further by examining the electronic properties of relevant atoms involved in the exchange process.

We computed the LDOS, Fig. 5, for the exchange and top hopping mechanisms for diffusion between MES C8 and C5. We plotted the LDOS for the combined s and p orbitals of the Ga atom in heterodimer at the transition site (highest energy point) for both top hopping and exchange diffusion. For exchange diffusion, the Ga atom in the heterodimer has fewer states available in the lower energy (−10.5 eV to −12.5 eV) region and we observe a shift to the right in overall states compared to top hopping, especially near the Fermi energy. The additional states at lower energies for top hopping correspond to the low energy barrier for diffusion.

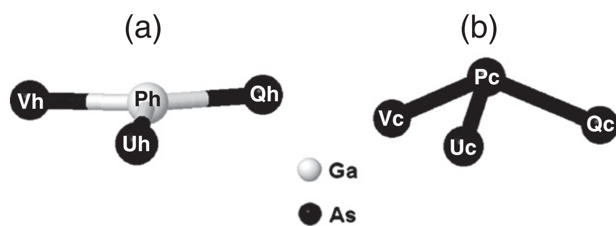

Fig. 4. In the GaAs (001)-$c(4\times4)$-hd reconstruction (a) the Ga atom of the heterodimer, Ph (from Fig. 1) bonds with the two sub-surface As atoms, Vh and Uh, and the As atom in the heterodimer, Qh. The structure and angles are similar to those of a planar configuration, as occurs in sp^2 hybridization. In the GaAs (001)-$c(4\times4)$-ss reconstruction (b) an As atom replaces the Ga atom and the same bonds form a structure which appears to be a tetrahedral configuration, as occurs in a sp^3 hybridized bulk material.

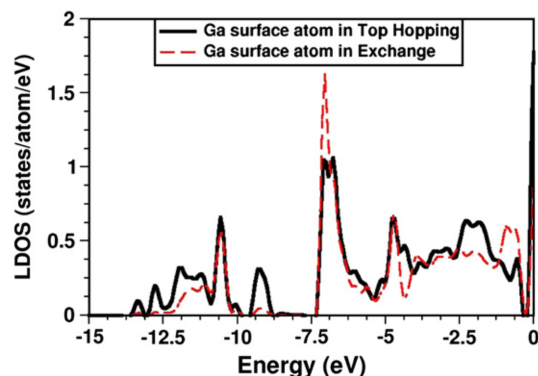

Fig. 5. Local density of states for the Ga atom of the surface edge heterodimer (Ga–As) at the highest energy point during top hopping and exchange diffusion of a Ga adatom between minimum energy sites C8 and C5. We observe a shift in the density of states to the right (in the range −2.5 eV to −1 eV) for the exchange mechanism correlated to a higher diffusion barrier compared to that for top hopping.

5. Summary

We have studied the energetics of a Ga adatom on the GaAs(001)-$c(4\times4)$-hd reconstruction using first principles calculations. We calculated structural differences between the $c(4\times4)$-ss and the $c(4\times4)$-hd reconstructions. MES for a Ga adatom on the $c(4\times4)$-hd surface were identified by computing the PES of the reconstruction. Energy barriers for diffusion of Ga adatom between neighboring MES were calculated for diffusion by way of top hopping and exchange mechanisms. We proposed two unique paths for diffusion of Ga adatom between the global minimum sites of two neighboring unit cells. We have found a correlation between the higher diffusion energy barrier for exchange mechanism compared to top hopping with differences in the LDOS of relevant atoms involved in the diffusion process.

Acknowledgments

The authors are grateful to the Ohio Supercomputer Center (OSC) for providing the computing resources. We acknowledge the financial support by the National Science Foundation (#DMR 0705464 and #CNS 0855134) and the Wright Center for PVIC.

References

[1] S. Adachi, GaAs and Related Materials: Bulk Semiconducting and Superlattice Properties, World Scientific, Singapore, 1994, p. 339.
[2] B.A. Joyce, D.D. Vvedensky, Mater. Sci. Eng. R 127 (2004) and references therein.
[3] A. Kley, P. Ruggerone, M. Scheffler, Phys. Rev. Lett. 79 (1997) 5278.
[4] K.A. Fichthorn, Y. Tiwary, T. Hammerschmidt, P. Kratzer, M. Scheffler, Phys. Rev. B 83 (2011) 195328.
[5] S.V. Khare, R.V. Kulkarni, D. Stroud, J.W. Wilkins, Phys. Rev. B 60 (1999) 4458.
[6] A. Ramstad, G. Brocks, P.J. Kelly, Phys. Rev. B 51 (1995) 14504.
[7] M. Sauvage-Simkin, R. Pinchaux, J. Massies, P. Calverie, N. Jedrecy, J. Bonnet, I.K. Robinson, Phys. Rev. Lett. 62 (1989) 563.
[8] J.E. Northrup, S. Froyen, Phys. Rev. B 50 (1994) 2015.
[9] J.E. Northrup, S. Froyen, Phys. Rev. Lett. 71 (1993) 2276.
[10] T. Ohno, Thin Solid Films 272 (1996) 331.
[11] J.G. LePage, M. Alouani, D.L. Dorsey, J.W. Wilkins, P.E. Blöchl, Phys. Rev. B 58 (1998) 1499.
[12] A. Ohtake, J. Nakamura, S. Tsukamoto, N. Koguchi, A. Natori, Phys. Rev. Lett. 89 (2002) 206102.
[13] M. Takahasi, J. Mizuki, Phys. Rev. Lett. 96 (2006) 055506.
[14] G. Kresse, J. Hafner, Phys. Rev. B 47 (1993) 558.
[15] G. Kresse, Thesis, Technische Universiät Wien, 1993.
[16] G. Kresse, J. Furthmüller, Comput. Mater. Sci. 6 (1996) 15.
[17] G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996) 11169.
[18] P. Hohenberg, W. Kohn, Phys. Rev. 136 (1964) B864;
W. Kohn, L.J. Sham, Phys. Rev. 140 (1965) A1133.
[19] E. Kaxiras, Comput. Mater. Sci. 6 (1996) 158.
[20] D. Vanderbilt, Phys. Rev. B 41 (1990) 7892.
[21] G. Kresse, J. Hafner, J. Phys. Condens. Matter 6 (1994) 8245.
[22] H.J. Monkhorst, J.D. Pack, Phys. Rev. B 13 (1976) 5188.
[23] J.L. Roehl, A. Kolagatla, V.K.K. Ganguri, S.V. Khare, R.J. Phaneuf, Phys. Rev. B 82 (2010) 165335.
[24] Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, Vol. 17a, Springer-Verlag, Berlin, 1982.
[25] M. Methfessel, A.T. Paxton, Phys. Rev. B 40 (1989) 3616.
[26] H. Jónsson, G. Mills, K.W. Jacobsen, Classical and Quantum Dynamics, in: B.J. Berne, et al., (Eds.), Condensed Phase Simulations, World Scientific, Singapore, 1998, p. 385.
[27] L.L. Wang, S.V. Khare, V. Chirita, A.A. Rockett, D.D. Johnson, A.I. Frenkel, N.H. Mack, R.G. Nuzzo, J. Am. Chem. Soc. 128 (2006) 131.