Defect creation by low-energy ion bombardment on GaAs (001) and Ge (001) surfaces

A. Kuronen, a,1 J. Tarus, b K. Nordlund b

a Helsinki University of Technology
Laboratory of Computational Engineering
P.O.Box 9400, FIN-02015 HUT, FINLAND
b University of Helsinki, Accelerator Laboratory
P.O.Box 47, FIN-00014 University of Helsinki, FINLAND

Abstract

We have studied the ion beam - surface interactions with the classical molecular dynamics simulation method. The properties of the GaAs (001) surface predicted by the potential model were investigated. The structure and amount of defects created on the GaAs (001) and Ge (001) surfaces under 50 eV Ga and Ge ions, respectively, were investigated and compared. The defect creation for the GaAs system was found to differ considerably from that of the Ge system. Since Ga, As, and Ge have similar masses this illustrates the importance of chemical effects on damage production in low-energy ion irradiation.

Key words: Radiation defects, surfaces, computer simulation

1 Introduction

The interaction between low-energy (<1 keV) ion beams and surfaces has gained considerable interest due to applications in thin film growth (1).

Due to the complexity of the processes in ion-beam–material interactions one has to resort to computational methods in modeling the phenomena. Interaction of low-energy ion beams with elemental semiconductor surfaces has been previously investigated using the classical molecular dynamics (MD) method

1 Corresponding author, email address anti.kuronen@hut.fi

Preprint submitted to Elsevier Preprint 12 October 1998
(See ref. (2) and references therein.) However, there seems to be no published studies on interaction between low-energy ions and compound semiconductor surfaces using dynamical simulations.

The objective of the present work is to study the interaction between the $2 \times 1$ and $2 \times 4$ reconstructed (001) As-rich surface of GaAs and 50 eV gallium ions incident on the surface using MD simulations. The number of defects in the sample is determined. To clarify chemical effects on damage production the defect creation on the $2 \times 1$ reconstructed Ge (001) surface was also investigated and compared to the GaAs surface bombardment.

2 Computational details

In this work, the Tersoff many-body potential was employed. For Ga–Ga, Ga–As, and As–As interaction the parameter set obtained by Sayed et al. (3) was used. For of germanium the parametrization is from ref. (4). The interatomic interaction at small separations was described by a pair potential calculated by the program package DMOL (5; 6). This was smoothly joined to the Tersoff potential at $r = 1.6 \, \text{Å}$.

Electronic slowing down was included as a nonlocal frictional force for all atoms having kinetic energies larger than 10 eV. The electronic stopping power was calculated by the program TRIM (7).

In the surface reconstruction and cascade simulations a simulation cell consisting of $8 \times 8 \times 6$ atoms was used. The total number of atoms was 3072 and 3040 for the $2 \times 1$ and $2 \times 4$ surface structures, respectively. The equilibrium configurations for the two surface reconstructions were calculated by starting from an ideal dimer-row structure and simulating this for 2 ps at 300 K. After this the system was quenched to 0 K using a quench rate of 0.15 K/fs. Atomic configurations obtained this way were used as the initial state for the cascade simulations.

In the cascade simulations a Ga (or Ge) atom was placed 4 Å above the simulation cell surface and was given a kinetic energy of 50 eV perpendicular to the surface. The time evolution of the system was followed for 4 ps during which the extra kinetic energy was dissipated by scaling the velocities of the atoms at the cell borders. After this the system temperature was quenched to zero with a rate of 0.015 K/fs.

The number of defects (vacancies, interstitial atoms, adatoms, sputtered atoms and antisite defects) were determined from the quenched configuration using the Wigner-Seitz (WS) cell method (8). In this method a vacancy is identified
when a primitive cell of the lattice is empty and an interstitial or interstitials when there are more than one atom in a cell. An atom is declared as an adatom when its distance from the surface is larger than 0.7 Å but smaller than the potential cut-off (3.6 Å for GaAs and 3.1 for Ge). An atom that has escaped the surface beyond the potential cut-off distance is labeled sputtered. In an antisite defect the atomic identity of a WS cell has changed.

3 Results and discussion

In the preliminary simulations the GaAs (001) surface was unstable if the parameter set of Sayed et al. was used. Stable surfaces were achieved when the \( \lambda_3 \) parameter values were reduced by multiplying them with a scaling factor \( \alpha \). Using scaling parameter values \( \alpha = 0 \ldots 0.3 \) the surface was stable up to 1000K. It should be noted that the equilibrium properties (lattice constant, cohesion energy, bulk modulus and elastic constant \( C' \)) used in ref. (3) to determine the parameter set are not affected by the scaling of the \( \lambda_3 \) parameter.

In this work, the most simple reconstruction of the GaAs (001) surface, the \( 2 \times 1 \) dimerization, was studied. In addition, the three-As dimer \( 2 \times 4 \) reconstruction (9) was also studied in order to gain information from the effect of surface structure on the damage.

The bond length obtained for the As-As dimer was 2.63 Å for the \( 2 \times 1 \) reconstruction and 2.64 Å for the \( 2 \times 4 \) reconstruction compared to the bulk bond length of 2.45 Å. The gain in energy of dimerization as compared to unreconstructed surface was 0.7 eV. These results are in fair agreements with density-functional calculations (10). The relaxations of atomic layers – as illustrated in fig. 1 – are qualitatively similar to those in silicon (2).

Cascade simulations were performed for different values of the scaling factor \( \alpha \). At low values (0–0.3) the number of different defects depended only very slightly on the scaling factor (see Fig. 2.) With these scaling factor values the surface (for both reconstructions) was stable.

In Table 1 the number of different defect species after quenching are given. The number of As vacancies is larger than Ga vacancies, probably because the surface is As-rich. As the number of Ga interstitial atoms includes the recoiling Ga atom there are more of them than As interstitials. This could also explain the larger tendency of Ga atoms to sputter. Finally, it can be seen that there are no large differences between the \( 2 \times 1 \) and \( 2 \times 4 \) cases.

The number of defects after quenching can be seen in Table 2 where the results for Ge and GaAs are compared. In GaAs the number of interstitial
atoms is considerably lower than in Ge. On the other hand more adatoms and sputtered atoms are created in bombardment of GaAs than of Ge. This could indicate that interstitial atoms are not favored in GaAs but the defect structures are finally formed on the surface of the substrate. By inspecting final atomic configurations it was observed that in most cases the As adatoms are created by the displacement of a dimer As atom creating also a vacancy on the surface and a buckled dimer row. This was not observed in the case Ge.

Fig. 3 shows the time dependence of the defects during the simulation. The number of interstitial atoms in GaAs rises to its maximum and reaches a constant value at about 400 fs. On the other hand, the number of other defect species—especially vacancies and adatoms—reach their equilibrium value only after 1000 fs which longer than in the case of Ge (see inset of Fig. 3). The time dependence of vacancies in and adatoms in GaAs is dominated by the number corresponding As defects.

In conclusion, we have studied interaction between low-energy ion-beams and As-rich GaAs (001) surface. The number of defects caused by 50-eV Ga-ion bombardment was calculated and compared with the results obtained for 50-eV self-bombardment of Ge the (001) surface. The total number of defects observed in GaAs and Ge was the same but the defects were distributed among the defect species in a different way. Moreover, the time dependence of the number adatoms and vacancies was different for GaAs and Ge. Since Ge and GaAs are expected to behave very similarly from a ballistic point of view, the differences between damage production in them illustrate the role chemical effects can have in low-energy ion irradiation.
References


[8] Since the diamond crystal structure is not a Bravais lattice, the cells centered at the lattice atoms are strictly speaking Voronoy polyhedra. See e.g. N. W. Ashcroft, N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia 1976), ch. 4.


Table 1
Number of defects after quenching for the two GaAs surface reconstructions studied. In both cases the $\lambda_3$ scaling factor $\alpha = 0.125$ was used. Results are given for different sublattices (vacancies and antisites) or atomic species (interstitials, adatoms, and sputtered atoms) (column 'Comp'.).

<table>
<thead>
<tr>
<th>Surface</th>
<th>Comp.</th>
<th>Vacancies</th>
<th>Interstitials</th>
<th>Adatoms</th>
<th>Sputtered</th>
<th>Antisites</th>
</tr>
</thead>
<tbody>
<tr>
<td>2×1</td>
<td>Ga</td>
<td>0.24±0.03</td>
<td>0.63±0.04</td>
<td>0.40±0.04</td>
<td>0.06±0.02</td>
<td>0.03±0.01</td>
</tr>
<tr>
<td></td>
<td>As</td>
<td>0.54±0.05</td>
<td>0.23±0.03</td>
<td>0.45±0.05</td>
<td>0.03±0.01</td>
<td>0.19±0.03</td>
</tr>
<tr>
<td>2×4</td>
<td>Ga</td>
<td>0.27±0.04</td>
<td>0.69±0.04</td>
<td>0.34±0.04</td>
<td>0.10±0.02</td>
<td>0.03±0.01</td>
</tr>
<tr>
<td></td>
<td>As</td>
<td>0.62±0.06</td>
<td>0.24±0.03</td>
<td>0.46±0.05</td>
<td>0.06±0.02</td>
<td>0.16±0.03</td>
</tr>
</tbody>
</table>

Table 2
Number of defects after quenching for GaAs and Ge 2×1 reconstructions. Results for GaAs are calculated using scaling factor $\alpha = 0.125$.

<table>
<thead>
<tr>
<th>System</th>
<th>Vacancies</th>
<th>Interstitials</th>
<th>Adatoms</th>
<th>Sputtered</th>
<th>Events</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ga $\rightarrow$ GaAs</td>
<td>0.78±0.06</td>
<td>0.85±0.05</td>
<td>0.85±0.06</td>
<td>0.09±0.02</td>
<td>200</td>
</tr>
<tr>
<td>Ge $\rightarrow$ Ge</td>
<td>0.78±0.06</td>
<td>1.26±0.04</td>
<td>0.50±0.06</td>
<td>0.023±0.011</td>
<td>210</td>
</tr>
</tbody>
</table>
Fig. 1. The longitudinal positions of the atomic layers of the $2 \times 1$ (solid line) and $2 \times 4$ (dotted line) reconstructions of the GaAs (001) surface. Narrow lines correspond to the bulk-like layer positions.

Fig. 2. Dependence of different defects on the scaling factor of the $\lambda_3$ parameter of the Tersoff model potential for GaAs.
Fig. 3. Time dependence of the number of different defects for the 2×1 GaAs surface during the simulation. The inset shows the time dependence for Ge.