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Group V adsorbate structures on vicinal Ge(001) surfaces determined from the optical spectrum

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Vicinal Ge(001) is the standard substrate for the fabrication of high-performance solar cells by metal-organic vapour phase epitaxy, where growth of the III-V material on single domain Ge surfaces, with a single dimer orientation, minimizes the formation of anti-phase domain defects. Reflectance anisotropy spectroscopy has proved to be a powerful and sensitive optical probe of such anisotropic surface structures, but moving beyond fingerprinting to atomic structure determination from the optical spectra has been held back by the high computational cost. It is shown that an empirical, local-orbital-based hybrid density functional theory approach produces very good agreement between the theory and the experiment for (2×1) -As and (2×1) -Sb structures grown on vicinal Ge(001). These results, when taken together with previous work on Si interfaces, show that this computationally efficient approach is likely to prove to be an important general technique for determining the structure of anisotropic semiconductor surfaces and interfaces by comparing the experimental and calculated optical spectrum. *Published by AIP Publishing.*
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Interest in the characterization of the electronic and optical response of single crystal Ge surfaces and interfaces has increased recently, driven by the search for higher efficiency photovoltaics,¹ higher mobility nanoscale devices,² and atomic-scale nanowire structures.³ Vicinal Ge(001) is the standard substrate for high-performance triple junction solar cells grown by metal-organic vapour phase epitaxy (MOVPE), where growth of the III-V material on single domain Ge surfaces, with a single dimer orientation, is used in order to avoid the formation of anti-phase domain defects. Ge(001) substrates offcut by 6° towards [110] are generally used, which form double height steps and thus predominantly single domain surfaces.

The single dimer orientation produced is anisotropic in the surface plane, allowing reflection anisotropy spectroscopy (RAS) to be used to probe the linear optical response of the surface region. Optical transitions between filled and empty electronic states of both the surface and bulk present a challenge to *ab initio* calculations and, experimentally, in distinguishing the much smaller surface signal from the bulk response.⁴ However, for suitable systems, RAS is highly sensitive to surface atomic structure as recent work on Si(111)-(5 × 2)-Au and related structures has shown.^{5,6}

RAS measures the difference, at a near-normal angle of incidence, in the reflection of light polarized along two orthogonal axes in the surface plane, normalized to the mean reflection. This is a spectroscopic ellipsometry technique adapted to measure only the anisotropy in the optical response. RAS is surface and interface sensitive when the bulk optical response is isotropic and the symmetry of the surface or interface structure is lower, possessing at the most a two-fold rotation axis.^{4,7} RAS is an ideal tool for probing structure at the (001) surfaces of Si, Ge, and III-V semiconductors, since atoms at those

surfaces break the isotropic symmetry of the bulk cubic structure by dimerizing. However, for Si and Ge, singular surfaces normally produce two equal domain populations of orthogonal dimers, nulling the signal, but vicinal surfaces can form a single or a predominant domain, allowing a RAS response to be measured.

While there have been many RAS studies of Si(001) surfaces, there have been very few studies of Ge(001), with recent work focusing on *in situ* MOVPE studies, where RAS has unique advantages.^{8–11} Regarding calculations of the spectral response, the situation is similar. Recently, we have calculated the optical response of some Si(001) and Ge(001) surfaces using a local-orbital-based hybrid density functional theory (DFT) approach.¹² The results were very promising and included a prediction of a large change in the RAS response on adsorption of Sb to form Ge(001)-(2 × 1)-Sb. Adsorption of group V elements on the Ge(001) surface is an important consideration in the fabrication of the triple junction solar cell material mentioned above.^{1,11}

In this work, hybrid DFT calculations are compared with experimental RAS measurements of Ge(001)-(2 × 1)-Sb and with previous experimental work on Ge(001)-(2 × 1)-As by Brückner *et al.*¹¹ Agreement between theory and experiment is very good, which is strong evidence that accurate atomic structures, and valence and conduction band energies and dispersions, have been produced by the empirical hybrid DFT approach. Atomic structures are in agreement with previous DFT studies, and the main optical features arise from transitions between electronic states on the dimer atoms and the Ge atoms bonded to the dimers. It is also shown that the Sb dimer bond is formed parallel to the step edge and the original Ge dimer bond direction on the vicinal surface, in contrast to the singular surface, which forms Sb dimer bonds in the orthogonal orientation.¹³ The steps and the narrow terraces of the 6° offcut substrates appear to favour a parallel orientation on adsorption of elemental Sb.

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Samples were cut from As-doped, 0.05–0.25 Ω cm resistivity vicinal Ge(001) wafers, offcut 6° towards either [111] or [110]. Procedures for producing clean, well-ordered sample surfaces have been described previously.¹² The LEED patterns obtained showed the vicinal surface spot splitting expected and, for the [111] offcut, a $(1 \times 2)/(2 \times 1)$ pattern, with no dominant domain, while the [110] offcut was predominantly single domain, in agreement with previous work.^{8–10} Antimony was evaporated onto the sample using a low temperature effusion cell. After deposition, the sample was annealed for 15 min at 680 K to remove excess Sb and form the (2×1) -Sb structure.

A visible/near-IR RAS system, operating down to ~ 0.4 eV (Ref. 14), was used, which employs a calcium fluoride photoelastic modulator (PEM) to change the polarization state of the light.¹⁵ The poorer signal-to-noise ratio below ~ 1 eV is associated with the InAs detector. The spectrometer measures the difference in reflectance, at near normal incidence, of light linearly polarized in two orthogonal directions in the surface plane

$$\frac{\Delta r}{r} = 2 \frac{r_x - r_y}{r_x + r_y}, \quad (1)$$

where r_x and r_y are the complex Fresnel reflection coefficients for the surface for light polarized in the x and y directions. The real part is measured in this work, with the steps and dimer bonds parallel to the x direction.

The local-orbital, hybrid DFT approach was used, first, to calculate minimum energy crystallographic and electronic structures and, second, to calculate the linear optical response and the reflection anisotropy (RA) spectra. The principal advantage of using a local orbital basis is computational efficiency. The exchange-correlation potential contains a weighted mixture of Fock exchange and conventional exchange correlation functionals. The importance of Fock exchange is that it widens the semiconductor band gap, relative to conventional DFT functionals. The weight of Fock exchange is adjusted so that the predicted bulk optical gap matches experiment and reproduces the bulk dielectric function. Very good agreement is obtained for both Si and Ge, when the relative weight of the Fock exchange functional is fixed at 5%.^{12,16} When calculating optical excitations using DFT methods, electron and hole potentials and the omission of electron–hole interactions are approximated using the *GW* and Bethe–Salpeter equation (BSE) approach, with the inverse dielectric function screening the Fock exchange. Surfaces and the underlying bulk structure must be represented by slabs containing a large number of atoms, and high k -point densities are often necessary when calculating the optical spectra. Consequently, the BSE method has been applied very sparingly to the calculation of RA spectra.¹⁷ The approach used here is an alternative, empirical approach, which addresses the DFT band gap problem and the electron-hole interaction.

The McIntyre–Aspnes 3-layer model¹⁸ is used to relate the calculated bulk and surface optical susceptibilities to the RAS response given by Equation (1)

$$\text{Re} \frac{\Delta r}{r} = 2kd \text{Im} \frac{(\Delta\chi_{xs}^i \chi_b^r - \Delta\chi_{xs}^r \chi_b^i)}{|\chi_b|^2}, \quad (2)$$

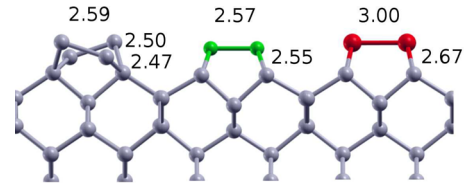


FIG. 1. Hybrid DFT minimum energy structures: left, Ge(001)- $c(4 \times 2)$, center, Ge(001)- (2×1) -As, and right, Ge(001)- (2×1) -Sb. Bond lengths are given in angstroms.

where r and i refer to the real and imaginary parts, the wave-vector magnitude is k , d is the surface region thickness, $\Delta\chi_{xs}(\omega)$ is the anisotropy in the surface excess susceptibility, and $\chi_b(\omega)$ is the bulk susceptibility (see [supplementary material](#) for more detail).

The minimum energy structures are shown in Fig. 1. The half-filled dangling bond states on Ge(001) reconstruct to form asymmetric dimers, comprising a lower filled lone pair and an upper empty lone pair. For Group V adsorbates, symmetric dimers are formed with two filled lone pairs. For clean Ge(001) surface reconstructions, there is good agreement between the theory and the experiment, with the observed structures being the most stable DFT structures.^{12,19,20} At room temperature, there are co-existing local patches of buckled, asymmetric dimers with different arrangements, producing (2×1) , $c(4 \times 2)$, and $p(2 \times 2)$ symmetries, with a (2×1) pattern dominating the LEED response. The Ge(001) crystallographic and electronic structures resulting from hybrid DFT energy minimization calculations have been reported previously.¹² The experimental optical spectra from different studies are very similar, all having a minimum in the range of 1.8–2.0 eV, another minimum at 3.0 eV, and maxima around 2.2 and 4.2 eV, the E_1 and E_2 critical points of bulk Ge.^{9,10} The calculated optical response for the $c(4 \times 2)$ and $p(2 \times 2)$ structures, using the hybrid DFT approach, is compared with the experiment in Fig. 2, where it can be seen

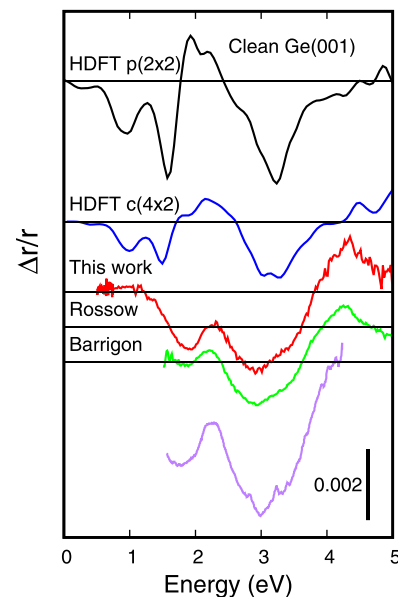


FIG. 2. RA spectra of single domain Ge(001). The black and blue lines depict the $p(2 \times 2)$ and $c(4 \times 2)$ calculations, respectively (scaled by $\times 0.2$). The experimental results from this work (red line), Rossow *et al.*⁹ (green line, scaled by $\times 2$) and Barrigon *et al.*¹⁰ (purple line), are shown below the calculations. The horizontal lines are the zero line of each spectrum.

that the spectral lineshape is well reproduced, although the reduced intensity of the ~ 2 eV peak observed results in an almost entirely negative-going experimental spectrum.

Care is required in the detailed interpretation of the spectra due to possible contributions from the step structure and surface modified bulk states of the vicinal offcut. Comparison of the experimental double-domain response with the predominantly single domain response reveals that significant differences only occur below 1.8 eV, indicating that the anisotropic surface state response above 1.5 eV is masked by transitions associated with the 6° offcut (see Fig. S1 in the [supplementary material](#)). Previous experimental results from the clean surface^{9,10} are dominated by the step structure and surface modified bulk states of the vicinal offcut.

Interpretation is clearer below the 1.5 eV cut-off of previous RAS studies. There appears to be a small experimental feature at 0.7–0.9 eV, which is also seen in the calculated response of the $c(4 \times 2)$ and $p(2 \times 2)$ structures (Fig. 2). The surface band structures calculated for the clean $p(2 \times 2)$ structure, and the group V adsorbate structures, are shown in Fig. 3. The upper figure shows the surface band projections onto the Ge asymmetric dimer up and down atoms (green squares and red circles, respectively), and the projections onto the Ge atoms bonded to dimers (blue squares). The small feature in the calculation is associated with transitions between the occupied surface state on the up atom of the Ge

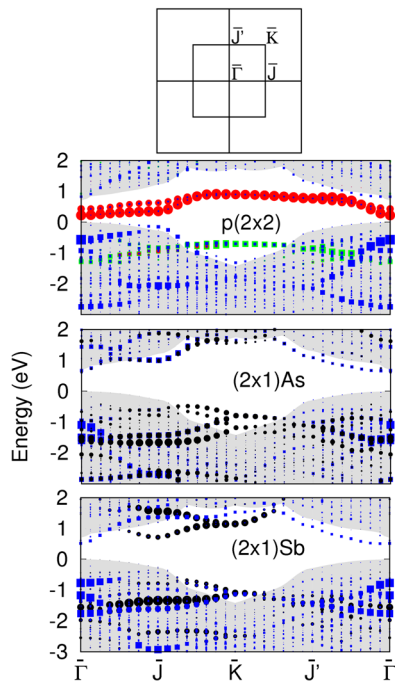


FIG. 3. The $p(2 \times 2)$ surface Brillouin zone (SBZ) and the electronic structure of Ge(001)- $p(2 \times 2)$ (upper) and (b) Ge(001)- (2×1) -As (middle) and Ge(001)- (2×1) -Sb (lower). The surface unit cell of (2×1) structures has been doubled to a (2×2) supercell. The Ge bulk band structure, projected onto the SBZ, is shown by shading. The surface band structure is projected onto the dimer atoms and Ge atoms bonded to dimer atoms. Upper: surface band projections onto the Ge dimer up and down atoms (green squares and red circles, respectively) and the projections onto Ge atoms bonded to dimer atoms (blue squares). The size of symbols reflects the degree of localisation on surface atoms. Middle: band projections onto As dimer atoms (black circles) and Ge atoms bonded to dimer atoms (blue squares). Lower: band projections onto Sb dimer atoms (black circles) and Ge atoms bonded to dimer atoms (blue squares).

dimer and the empty surface state on the down Ge atom. Due to the small size of the feature, further experimental work is needed before it can be concluded that these transitions are being observed.

Interpretation turns out to be much simpler for group V adsorbates on Ge(001). It is generally agreed by both the experiment^{13,21} and the theory^{12,22–24} that the (2×1) -As and (2×1) -Sb structures form symmetric dimers, in contrast to the asymmetric Ge dimers of clean surface. In addition, the surface x-ray standing wave study of the singular double-domain surface showed that the Sb dimers form at 90° to the Ge dimer orientation.¹³ Here, the LEED patterns of the predominantly single domain structures of clean Ge(001) and Ge(001)- (2×1) -Sb show that both the Ge and Sb dimer bond directions are parallel to the step edges (see Fig. S2 in the [supplementary material](#)). This requires a considerable reorganization of the Ge atoms on Sb adsorption. It has been shown that this can occur for the analogous (2×1) -As surface, where different surface structures are formed depending on preparation conditions.^{11,25,26} However, the same (2×1) -Sb preparation conditions are used here as in previous singular Ge(001) work,¹³ leading to the conclusion that the parallel Sb dimer orientation is a consequence of the aligned steps and narrow terraces (~ 7 atoms wide) of the vicinal substrate. The structure of adsorbates determined on the wide terraces of singular substrates cannot be assumed to apply to the narrower terraces of vicinal substrates.

Figure 4 shows the experimental¹¹ and calculated RA spectra of Ge(001)- (2×1) -As and of Ge(001)- (2×1) -Sb, which differ significantly from the clean surface spectra of Fig. 2. The experimental RA spectra of the As and Sb systems are very similar to each other and are dominated by a strong maximum and a strong minimum at ~ 2.0 eV and ~ 3.5 eV,

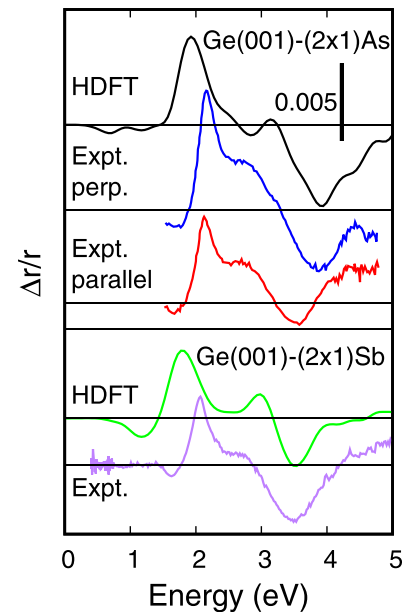


FIG. 4. RA spectra of Ge(001)- (2×1) -As (upper) and Ge(001)- (2×1) -Sb (lower). Upper: the black, blue, and red lines show the calculation, and the experimental response perpendicular (inverted) and parallel to the dimers, respectively (experimental data generated from Ref. 11). Lower: the green and purple lines show the calculation and the experimental response parallel to the dimers, respectively. The calculated RA spectra are scaled by $\times 0.2$. The horizontal lines are the zero line of each spectrum.

respectively, with the As features ~ 0.1 eV higher in energy than the Sb features. The spectral lineshapes are very well reproduced, which is strong evidence that accurate crystallographic, valence band, and conduction band structures have been produced by the empirical hybrid DFT approach.

The theory allows detailed interpretation of the optical spectra. The electronic band structures of Ge(001)-p(2×2), Ge(001)-(2×1)-As, and Ge(001)-(2×1)-Sb are compared in Fig. 3. The surface band structure changes significantly when the asymmetric Ge dimer atoms at the clean surface are replaced by group V atoms in symmetric dimers. Two nearly degenerate, occupied surface states localized on the dimers appear in the region of the J point, 1.5 eV below the valence band maximum (VBM). Two unoccupied surface states are also localized on the dimers, a little below the conduction band minimum. The increase in the surface state gap, which arises from the removal of most of the unoccupied dimer states from the gap (Fig. 3 upper, red circles), results in very little signal below 1.7 eV, with only a weak minimum appearing at ~ 1.0 eV. The calculations show that the peak at ~ 2 eV in the RA spectra of the group V surfaces is due to transitions between surface states primarily localized on the group V adatoms, with the external electric field aligned parallel to the dimer bonds. The dominant transitions between these states occur along the ΓJ and $J K$ lines in the Brillouin zone (Fig. 3, middle and lower, black circles). The nearly parallel bands localized on the group V atoms and the unoccupied surface states lying just below the bulk conduction band edge create a large density of states, resulting in a dominant optical response at ~ 2 eV.

RAS is a powerful and sensitive probe of anisotropic surface structures, but interpretation of the optical spectra beyond fingerprinting has been held back by the high computational cost. It has been shown that an empirical, local-orbital-based hybrid DFT approach produces very good agreement between the theory and the experiment for (2×1)-As and (2×1)-Sb structures grown on vicinal Ge(001). The major peaks observed in the optical response are found to be dominated by transitions between electronic states on the dimer atoms and, for the clean surface, the Ge atoms bonded to the dimers. As the same hybrid density functional works very well for Si, Ge, and GaP,²⁷ this computationally efficient empirical approach is likely to prove to be an important general technique for determining the structure of anisotropic semiconductor surfaces and interfaces by comparing the experimental and calculated optical spectrum.

See [supplementary material](#) for more detail on the hybrid DFT approach, the difference between the singular and vicinal Ge(001) optical response, and the LEED images of Ge(001)-(2×1) and Ge(001)-(2×1)-Sb.

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