Electron counting model and its application to island structures on molecular-beam epitaxy grown GaAs(001) and ZnSe(001)

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(Received 13 June 1989)

The principal reconstructions found on the low-index planes of GaAs and ZnSe can be explained in terms of a simple electron counting model. A surface structure satisfies this model if it is possible to have all the dangling bonds on the electropositive element (Ga or Zn) empty and the dangling bonds on the electronegative element (As or Se) full, given the number of available electrons. This condition will necessarily result in there being no net surface charge. The justification for this model is discussed. The GaAs(001)-(2×4) reconstruction is known to involve surface dimers. It is shown that a (2×4) unit cell with three dimers and one dimer vacancy is the smallest unit cell that satisfies the electron counting model for this surface. The electron counting model is used to explain the structure of islands imaged by scanning tunneling microscopy on the GaAs(001)-(2×4) surface. The model shows that island structures built up from complete (2×4) unit cells can be stable if they extend in the 2× direction, but not if they extend in the 4× direction. These island structures can also provide an explanation for the different step structures seen on GaAs(001) vicinal surfaces. Much less is known experimentally about step and island structures on ZnSe(001). Structures on this surface predicted by the electron counting model differ significantly from those found on GaAs(001).

INTRODUCTION

Molecular-beam epitaxy (MBE) growth of GaAs(001) is normally carried out under arsenic-rich conditions. This surface has recently been studied by scanning tunneling microscopy (STM),[1,2] which showed that the (2×4) reconstruction seen during growth arises from dimerization of the surface As atoms, with every fourth dimer missing. The surface is thus made up from blocks of three arsenic dimers separated in the 4× direction by rows of missing dimers as shown in Fig. 1. The experimental data supported the model that had previously been proposed by Chadi.[3] His total-energy calculations found the missing dimer model to be the lowest-energy structure for this surface. It is possible to understand the origin of this reconstruction from a simple electron counting model.[4] In this paper the justification for such a model will be discussed, and it will be shown that the principal reconstructions found on the low-index planes of GaAs can all be explained in this way.

A striking feature of the STM study of the GaAs(001)-(2×4) surface[1,2] was the structure of islands. They were found to be made up from complete (2×4) unit cells and to be many unit cells long in the 2× direction, but only one or two unit cells wide in the 4× direction. Thus, the islands had long step edges parallel to the 2× direction and short step edges parallel to the 4× direction. It was also found that steps found on a nominally flat (001) surface tended to run along the 2× direction. It is of increasing importance to understand the structure of islands and steps on the GaAs(001) surface as they can have a major impact on the growth of thin-layer superlattices, and the growth of tilted superlattices on vicinial surfaces.[5] The same electron counting model that can explain the nature of the (2×4) reconstruction can be used to consider possible island structures on the GaAs(001) surface. It is found that the observed island

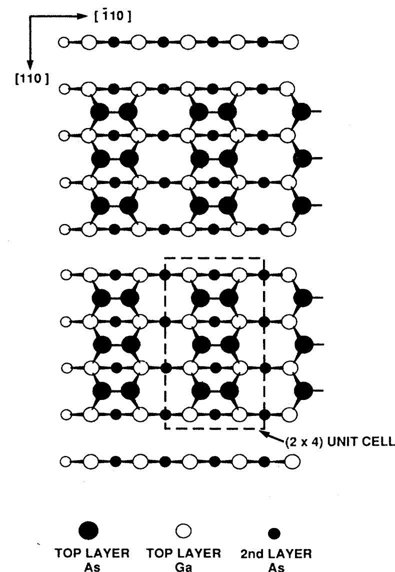

FIG. 1. The missing dimer structure of the GaAs(001)-(2×4) reconstruction as determined by STM results (Ref. 1) and total-energy calculations (Ref. 3).

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structures can be understood in these terms. The islands can then in turn affect the step structures seen on GaAs(001) vicinal surfaces.

There is increasing interest in MBE growth of wide-band-gap II-VI semiconductors such as ZnSe. The same electron counting model can also be applied to ZnSe, and there are interesting differences between the reconstructions on the (001) surfaces of these two materials which can be explained by this model. Although no experimental data on island and step structures on ZnSe(001) exist, it is instructive to predict the type of structures that we might expect to see and what effect they may have on the growth of ZnSe(001) on GaAs(001).

THE ELECTRON COUNTING MODEL

The atoms in both GaAs and ZnSe are sp^3 hybridized. In the bulk, two hybridized orbitals, one from each type of atom, combine to form a bonding and antibonding orbital. At the surface, some hybrid orbitals cannot form bonds; therefore, if no reconstruction occurs, partially filled sp^3 dangling bonds will remain. The energy levels of these dangling bonds can be estimated from the energies of the s and p atomic levels from which they are derived. These energies can then be compared with the conduction-band minimum and valence-band maximum of the bulk semiconductor. This is shown in Fig. 2 (data from Harrison[6]) where it can be seen that for both GaAs and ZnSe the dangling-bond energy level of the electropositive element (Ga or Zn) is in the conduction band, and should therefore be empty. The dangling-bond energy level for the electronegative element (As or Se) is in the valence band and should therefore be filled. In order to achieve this, electrons transfer from the dangling bonds of the electropositive element to the dangling bonds of the electronegative element. The electron counting model requires that a surface structure is found where the number of available electrons in the surface layer will exactly fill all dangling-bond states in the valence band, leaving those in the conduction band empty. If this condition is satisfied, then the surface will be semiconducting, whereas partially filled dangling bonds may lead to a metallic surface. The basic assumption of the electron counting model can be stated as follows.

(1) The lowest-energy structure is obtained with filled dangling bonds on the electronegative element (with V_n valence electrons) and empty dangling bonds on the electropositive element (with V_p electrons).

In order to apply this to the GaAs(001) surface, further assumptions on the nature of the reconstruction are required. These can be obtained from the STM images.[1,2] Thus, we will also assume the following.

(2) The surface forms a $(2\times N)$ reconstruction.

(3) The $2\times$ periodicity arises from the formation of surface dimers.

(4) The $N\times$ periodicity arises from missing surface dimers, leaving D dimers per unti cell where $D \leq N$.

We now count up the number of electrons required to satisfy these conditions and equate that with the number of electrons available in order to determine the relationship between N and D. Thus, from Fig. 3 each top layer dimer requires six electrons (two in each dangling bond and two in the dimer bond), making $6D$ electrons in total

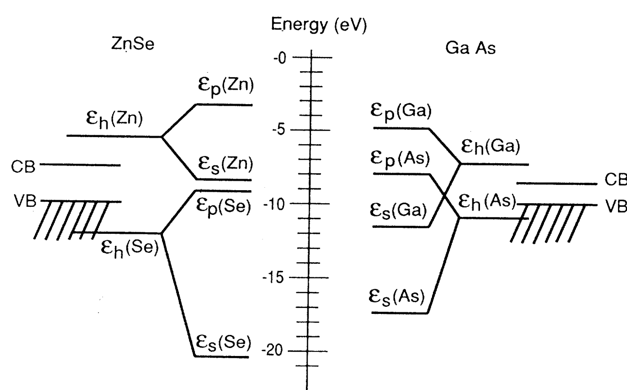

FIG. 2. The energy levels ε_h of the sp^3 dangling-bond states of GaAs and ZnSe. The energies are derived from the energies of the s and p orbitals, ε_s and ε_p, respectively. The Ga and Zn dangling-bond energies are above the conduction-band minimum (CB) and the As and Se dangling-bond energies are below the valence-band maximum (VB). The data are from Harrison (Ref. 6).

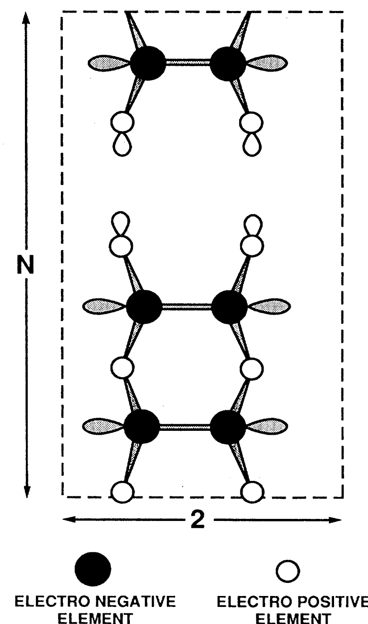

FIG. 3. The bonds and dangling bonds, both filled (shaded) and empty (open), for a $(2\times N)$ unit cell on the (001) surface of a polar semiconductor with the zinc-blende crystal structure, where the $N\times$ periodicity arises from missing dimers.

in the top layer. A total of $8D$ electrons are required to bond the dimers to the second layer of atoms. The number of electrons available from the top-layer atoms is $2V_nD$, and the number available from the second layer is $2V_pN/2$ electrons (since half of the total electrons from the second layer are involved in bonding to the third layer). Thus, a stable structure is obtained when

$$6D + 8D = 2V_nD + V_pN \ . \quad (1)$$

In the case of GaAs, $V_n = 5$ and $V_p = 3$. Thus,

$$4D = 3N \ .$$

The smallest unit cell that satisfies this condition is a (2×4) unit cell with three dimers and one missing dimer per unit cell. This structure for the (2×4) reconstruction agrees with the results of total-energy calculations[3] and STM experiments.[1,2] Thus, the removal of every fourth arsenic dimer is required in order to satisfy the electron counting model, and results in a semiconducting surface. The application of the electron counting model on this surface is based on sp^3-hybridized dangling bonds. Harrison[7] has suggested that on the (001) unreconstructed surface, where each atom has two sp^3 dangling-bond states, rehybridization can occur forming new dangling-bond states. However, in the case of the GaAs(001)-(2×4) surface, the rehybridization proposed in Ref. 7 is found not to be correct since the rehybridized orbitals cannot satisfy the electron counting model for the experimentally determined surface structure.

In the case of the selenium-rich (001) surface of ZnSe, $V_n = 6$ and $V_p = 2$. Thus, making the same assumptions as for GaAs(001), we find from Eq. (1) that $N = D$; that is, we expect a (2×1) reconstruction consisting of a complete layer of selenium dimers. In fact, this surface does form a (2×1) reconstruction,[8] and so it would appear that it is also consistent with the electron counting model. However, it should be noted that as yet there is no experimental proof that this surface forms dimers.

The analysis can also be applied to the gallium- or zinc-rich surfaces following the same four assumptions listed above. In this case, the surface dimers have empty dangling bonds and the dangling bonds in the arsenic or selenium layer, resulting from missing dimers, are filled. The $2\times$ periodicity arising from surface dimers is perpendicular to that on the arsenic or selenium surface, and so it is conventional to label the reconstruction as a $(N\times2)$. A stable structure is obtained when

$$2D + 8N = 2V_pD + V_nN \ .$$

The model thus predicts a (4×2) unit cell with three dimers and one missing dimer per unit cell for the GaAs(001)-Ga surface and a (1×2) complete layer for the ZnSe(001)-Zn surface. Experimentally, it is found that the GaAs(001)-Ga surface forms a (4×2) reconstruction which is thus consistent.[9] The ZnSe(001)-Zn surface forms a $c(2\times2)$ reconstruction.[8] If the assumption that this surface forms zinc dimers is correct, then a $c(2\times2)$ reconstruction is also consistent with the model. The $c(2\times2)$ periodicity will arise from a complete layer of zinc dimers where each dimer row is displaced by one spacing in the $2\times$ direction with respect to the previous dimer row. This is exactly equivalent to a (1×2) dimer structure as far as the electron counting model is concerned.

Experimentally, it is found that the arsenic-rich surface of GaAs(001) actually forms a mixture of (2×4) and $c(2\times8)$ reconstructions. STM images have shown that the $c(2\times8)$ reconstruction is made up from (2×4) unit cells where the rows of unit cells are displaced by a single spacing in the $2\times$ direction with respect to the previous row.[1] Again, this is exactly equivalent to the (2×4) reconstruction as far as the electron counting model is concerned. It is simply a matter of a different arrangement of the (2×4) unit cells on the surface. Similarly, the GaAs(001) gallium-rich surface forms a mixture of (4×2) and $c(8\times2)$ reconstructions.[9] Although no STM data are available for this surface, it is likely that the $c(8\times2)$ is also a different arrangement of (4×2) unit cells, and so the structure is consistent with the electron counting model. There are some other reconstructions seen on GaAs(001) apart from the (2×4) and (4×2) reconstructions. These include the $c(4\times4)$.[10,11] Their structure is not well understood, but they probably arise from different surface stoichiometries and may involve adsorbed overlayers.[10,11] They are most often seen as a result of different growth conditions. It remains to be seen whether or not they can be explained by the electron counting model.

Although the assumptions 2–4 above apply only to the (001) surfaces, the first assumption of the electron counting model is generally applicable. All the principal reconstructions found on the low-index planes of GaAs and ZnSe are consistent with the electron counting model (see Table I). The GaAs(111)A-Ga(2×2) reconstruction[13–15] is another example where surface vacancies (in this case single-atom vacancies as oppose to dimer vacancies) are created in order to allow the surface to become semiconducting. One in four of the surface gallium atoms is removed leaving three Ga dangling bonds in the surface layer. These can then donate their electrons to the three As dangling bonds in the layer below created by the removal of the gallium atom. This leaves the surface gallium dangling bonds empty and the arsenic dangling bonds filled.

Surface reconstructions of polar semiconductors have also been considered in terms of surface charge by Harrison.[7] In the case of GaAs, Harrison assumes that all arsenic dangling bonds are necessarily filled and all gallium dangling bonds are necessarily empty, due to their respective energy levels (see Fig. 2). This assumption is made irrespective of the surface structure, whether ideal or reconstructed. In general this leads to a net charge at the surface which sets up an electric field in the crystal. This is energetically unfavorable, and so a surface structure is found where there is no net surface charge. The condition for zero net surface charge turns out to be exactly the same as that required to satisfy the electron counting model. Thus, all structures which satisfy the electron counting model necessarily have zero net surface charge. There is usually a surface dipole associated with the reconstructions, but this does not result in an electric

TABLE I. Surface reconstructions of GaAs and ZnSe that are consistent with the electron counting model. The periodicities of the reconstructions on these surfaces are well known from diffraction data. Where there is strong experimental evidence supporting the particular structural model, it is indicated. LEED denotes low-energy electron diffraction.

Surface	Reconstruction	Experiment
GaAs(001)-As	(2×4) missing dimer model[a]	STM[b]
GaAs(001)-Ga	(4×2) missing dimer model	
ZnSe(001)-Se	(2×1) dimer model	
ZnSe(001)-Zn	$c(2\times2)$ dimer model	
GaAs(110)	(1×1)	c, STM[d]
ZnSe(110)	(1×1)	c
GaAs(111)*A*-Ga	(2×2) single-Ga-vacancy model[e]	LEED,[f] STM[g]
GaAs(111)*B*-As	(2×2) multiple-vacancy model[h]	

[a]Reference 3.
[b]Reference 1.
[c]In the case of the (110) surfaces, there have been many experimental structural determinations. See, for example, Ref. 17 and references therein.
[d]Reference 12.
[e]Reference 13.
[f]Reference 14.
[g]Reference 15.
[h]Reference 16.

field within the bulk of the crystal. Harrison[7] suggests that the most favorable structures would be those with no surface dipole. However, experimentally this is found not to be the case (Harrison's model would predict surface dipoles to be present for all the reconstructions listed in Table I). The surface dipole is difficult to calculate since it depends on the details of any surface relaxations which alter the interplanar spacing in the surface region.

The electron counting model has been used by others as a basis for models of MBE growth on GaAs(001) (Ref. 4) and ZnSe(001).[18] Here, the model will be extended to gain an understanding of the island and step structures that have been observed on the GaAs(001)-(2×4) surface.[2]

ISLAND AND STEP STRUCTURES

The formation of islands on the GaAs(001)-(2×4) surface extending along the 2× direction can be simply modeled. Starting from a perfect (2×4) surface a row of (2×4) unit cells is added, together with sufficient arsenic atoms in the missing dimer rows, so that all atoms in the island are fully bonded to the layer below (see Fig. 4). Thus, the atoms buried by the island are in bulklike configurations. As with the islands seen by STM,[2] the model island shown in Fig. 4 is made up from complete (2×4) unit cells. In order to determine the stability of the island in terms of the electron counting model, we consider an island that is infinite in the 2× direction and a single-unit-cell wide in the 4× direction. The number of electrons required in this structure and the number of available electrons can be counted for one unit of the island; that is, a single unit cell in the 2× direction and two unit cells in the 4× direction (since the island partially overlaps two unit cells of the main plane in the 4×

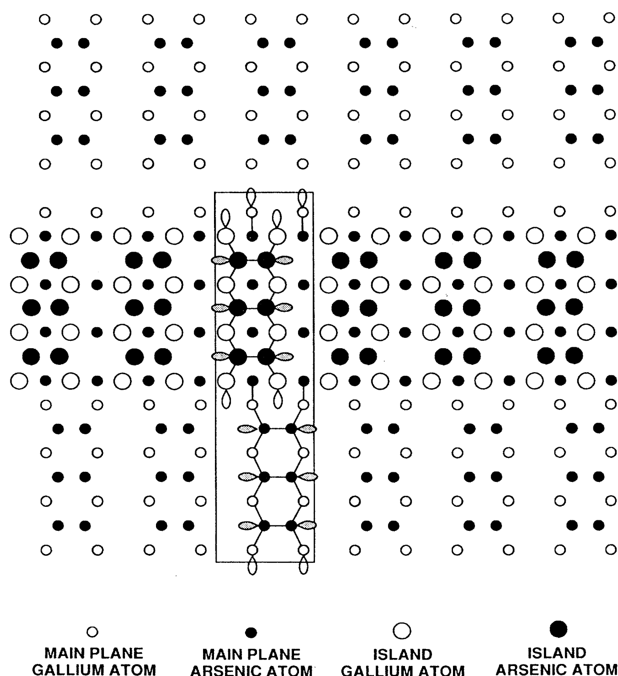

FIG. 4. An island on the GaAs(001)-(2×4) surface made up from complete (2×4) unit cells. It is infinite in length along the 2× direction (horizontal) and is one unit cell wide in the 4× direction (vertical). The bonding and dangling bonds are marked for one unit of the island structure. Some of the main plane Ga atoms have been left out in the island for clarity. This structure satisfies the electron counting model.

direction). This is shown in Fig. 4. It is found that for this structure, the electron counting model is satisfied. There is an excess of 1.5 electrons per unit cell along the top edge of the island which is exactly canceled by a deficit of 1.5 electrons per unit cell along the bottom of the island. This implies that in order to satisfy the electron counting model, charge must be transferred across the width of the island. This will result in an increase in electrostatic energy of the island through the separation of charge. However, a simple electrostatic calculation shows that the energy is at most of the order of 1 eV per unit cell of the island. This is smaller than the energy gained in allowing the 1.5 electrons to move from a gallium dangling-bond state to an arsenic dangling-bond state (see Fig. 2). This charge transfer should therefore not invalidate the electron counting model. There are two inequivalent locations for this island structure on the surface plane. The alternative location is obtained with the island placed one spacing lower in Fig. 4 with respect to the main plane. Both locations for the island satisfy the electron counting model.

An alternative island structure is shown in Fig. 5. Here, complete (2×4) unit cells are lined up along the $4\times$ direction, making the island one unit cell wide in the $2\times$ direction. As with the island structure shown in Fig. 4, sufficient arsenic atoms are added to the missing dimer rows of the main plane so that all atoms in the island are fully bonded to the layer below. For this island structure (Fig. 5) one unit of the island consists of a single unit cell in the $4\times$ direction and two unit cells in the $2\times$ direction (since the island partially overlaps two unit cells of the main plane in the $2\times$ direction). Again the number of electrons available can be counted, and compared with the number of electrons required in order to satisfy the electron counting model. In this case it is found that there is an overall deficit of three electrons per unit of the island, and, therefore, it is not possible to satisfy the electron counting model There is only one location for this island structure on the surface plane.

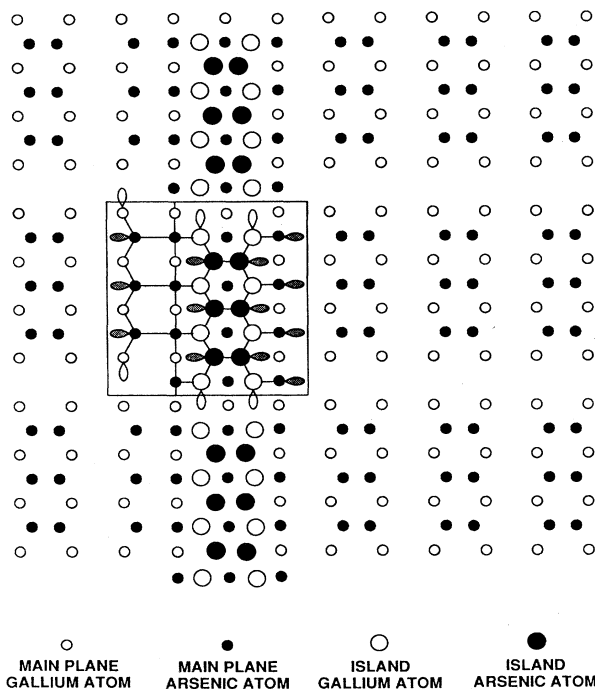

FIG. 5. An island structure on the GaAs(001)-(2×4) surface which is infinite in length along the $4\times$ direction (vertical) and one-unit-cell wide in the $2\times$ direction (horizontal). The bonding and dangling bonds are marked for one unit of the island structure. Some of the main plane Ga atoms have been left out in the island for clarify. This structure does not satisfy the electron counting model.

We therefore conclude from the electron counting model that islands made up from complete (2×4) unit cells extending in the $2\times$ direction should be stable, whereas islands made up from complete (2×4) unit cells extending in the $4\times$ direction should not. This is in agreement with the STM images of this surface[1,2] which show islands to extend in the $2\times$ direction but not the $4\times$ direction. The STM images show considerable disorder on this surface, including the island structures. They are not generally perfect straight rows of unit cells. However, the general trend is clear and can be understood from consideration of the electron counting model.

The structure of islands, as discussed above, results in a larger density of step edges parallel to the $2\times$ direction than parallel to the $4\times$ direction. A surface with a regular array of steps can be made by cutting a vicinal surface of a few degrees off the (001) orientation. There are two inequivalent vicinal (001) surfaces with steps parallel to $\langle 110\rangle$-type directions. The step edges can either run along the $[\bar{1}10]$ direction ($2\times$ direction) or along the [110] direction ($4\times$ direction). The structural order of these two different types of steps has been studied by Pukite *et al.*[19] by reflection high-energy electron diffraction (RHEED), and it was found that steps running parallel to the $2\times$ direction are straight over long distances, whereas the steps parallel to the $4\times$ direction are highly kinked. In order to try and understand the structure of steps on the two vicinal surfaces, we can consider the growth of islands on these surfaces. In the case of steps parallel to the $2\times$ direction, the addition of islands on the terraces will have little effect on the step edge since the islands will run parallel to the steps [Fig. 6(a)]. However, on a surface with steps running parallel to the $4\times$ direction, islands will tend to grow perpendicular to the step edges. The electron counting model suggests that it is favorable for the islands to grow out from the step edges [Fig. 6(b)]. This will result in a highly kinked step edge as observed by Pukite *et al.*[19] Thus, the structure of the islands on the GaAs(001)-(2×4) surface may be a major factor in determining the geometry of steps on this surface. This is, at least in part, supported by the STM images of the nominally flat (001) surface[2] where long step edges are seen parallel to the $2\times$ direction, and not parallel to the $4\times$ direction.

So far, there is no experimental evidence of island structures on the (001) surface of ZnSe. However, based on the dimer model for the Se-rich (2×1) surface dis-

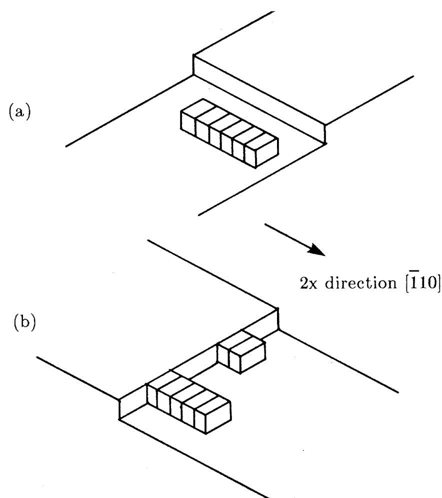

FIG. 6. The effect of island structure on stepped GaAs(001) surfaces under arsenic-stabilized growth conditions. The islands are built up from complete (2×4) unit cells. (a) The step edge is parallel to the length of the island, which leaves a straight step edge. (b) The step edge is perpendicular to the length of the islands resulting in a highly kinked step edge.

cussed above, we can use the electron counting model to determine which island structures, if any, might be stable. In this case we will consider islands made up from complete (2×1) unit cells extending in either the 2× ([$\bar{1}$10]) direction or the 1× ([110]) direction. The structure of an island extending in the 2× direction is shown in Fig. 7. The electron counting model shows that there are two electrons excess per unit of the island. Thus, this structure is not expected to be stable. However, the island extending in the 1× direction (Fig. 8) is stable according to the electron counting model provided excess charge of 0.5 electrons per unit of the island are transferred from the left to the right side of the island. The stable island structures expected on the ZnSe(001)-(2×1) surface are thus perpendicular to the stable island structures that are seen on the GaAs(001)-(2×4) surface. Presumably, the direction of straight step edges would also be perpendicular to those on the GaAs(001)-(2×4) surface.

It is possible to grow ZnSe under both Se- and Zn-rich conditions. The islands discussed above relate to Se-rich conditions. For growth under Zn-rich conditions [with a $c(2\times2)$ reconstruction] the electron counting model would predict stable island structures to form along the [$\bar{1}$10]. Thus, the islands on the Zn surface would be per-

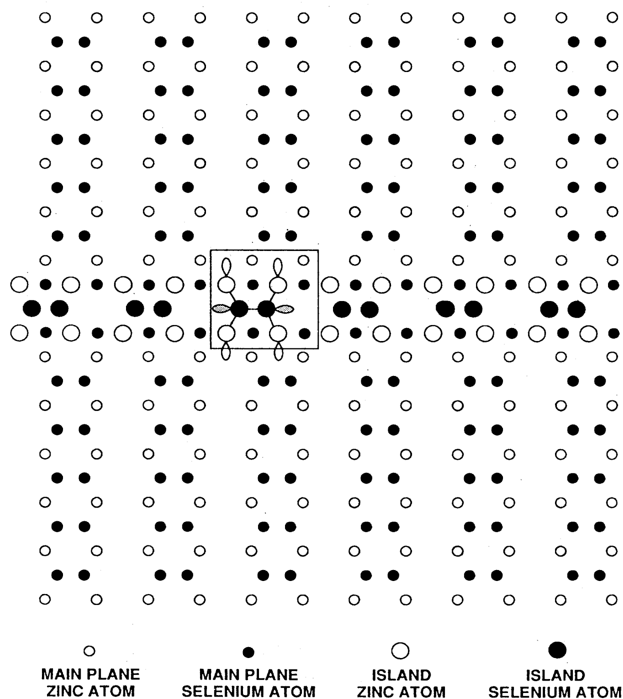

FIG. 7. A possible island structure on the ZnSe(001)-(2×1)-Se surface made up from complete (2×1) unit cells. It is infinite in length along the 2× direction (horizontal) and is one unit cell wide in the 1× direction (vertical). The bonding and dangling bonds are marked for one unit of the island structure. Some of the main-plane Zn atoms have been left out in the island for clarity. This structure does not satisfy the electron counting model.

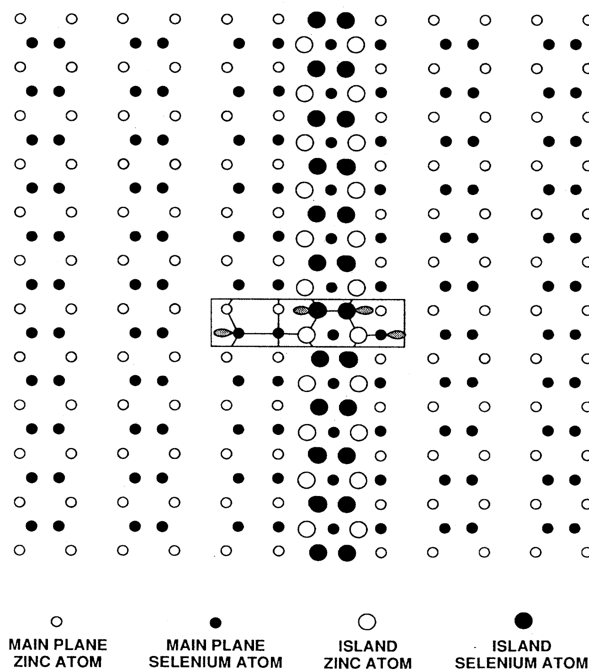

FIG. 8. A possible island structure on the ZnSe(001)-(2×1)-Se surface which is infinite in length along the 1× direction (vertical) and one unit cell wide in the 2× direction (horizontal). The bonding and dangling bonds are marked for one unit of the island structure. Some of the main-plane Zn atoms have been left out in the island for clarity. This structure satisfies the electron counting model.

pendicular to the islands on the Se surface. In both cases the islands are perpendicular to the surface dimers.

The structure of islands and steps on GaAs and ZnSe may have an influence on the growth of ZnSe(001) on GaAs(001). This may be particularly important for MBE growth of ZnSe on epitaxial GaAs(001) vicinal surfaces. Starting with a GaS(001)-(2×4) surface with steps parallel to the 2× direction, having a regular step structure, growth of ZnSe under zinc-rich conditions should result in a regular step structure in the ZnSe layer since the preferred step direction is the same in both layers. Growth of ZnSe under selenium-rich conditions might produce an irregular step structure since the preferred step orientations are perpendicular in the two layers.

CONCLUSION

The electron counting model can successfully explain the principal reconstructions found on the surfaces of GaAs and ZnSe. However, the model does not uniquely determine the surface reconstruction. In many cases, there are several possible structures which fit the model. However, any successful structural model must satisfy the electron counting model. It is also found that satisfying the electron counting model necessarily results in there being no net surface charge. The application of the electron counting model requires a knowledge of the energies of the dangling-bond states at the surface. They have been assumed to be sp^3 hybrid orbitals in all the cases considered.

The electron counting model is also able to explain the structure of islands seen on the GaAs(001)-(2×4) surface. Islands made up from complete (2×4) unit cells, extending infinitely along the 2× direction and only one unit cell wide in the 4× direction satisfy the electron counting model. This type of island structure has been seen by STM.[2] Islands extending in the 4× direction do not satisfy the electron counting model and have not been seen by STM. The observed island structure provides a possible explanation for the different step structures seen on vicinal surfaces where step edges parallel to the 2× direction are found to be straight, and step edges parallel to the 4× direction are found to be highly kinked.[19] The model also predicts the structure of islands on the ZnSe(001)-(2×1)-selenium surface. Stable islands are expected to extend along the 1× direction, that is perpendicular to those found on the GaAs(001)-(2×4) surface. Islands on the ZnSe(001)-c(2×2)-zinc surface are expected to be parallel to those on the GaAs(001)-(2×4) surface.

ACKNOWLEDGMENTS

I would like to thank C. van de Walle for many helpful discussions.

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