Clustering of Charged Adsorbates: Scanning Tunneling Microscopy Observations of Chlorine on Gallium-Rich GaAs(001)-*c*(8×2)

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The forces between adsorbates on metals are often repulsive due to dipole−dipole interactions. Electronegative adsorbates on semiconductors, however, sometimes form clusters, exhibiting attractive interactions even though the same dipole−dipole model should apply. Here we report observations with scanning tunneling microscopy of the clustering of chlorine chemisorbed on the gallium arsenide(001)-*c*(8×2) surface. For this system, the adsorbate has been found to have an anomalously high mobility; the clustering is therefore clearly energetically favored, rather than kinetically frozen. The clustering can be understood on a purely electrostatic basis. Because the Cl−Ga bonds are not normal to the surface, clusters more closely resemble an ionic crystal than an array of dipoles. Charging of the second-neighbor Ga of the Cl adsorbate enhances this effect.

I. Introduction

When very electronegative or electropositive atoms adsorb on metals, the charge transfer creates dipoles, and the adsorbates normally experience repulsive dipole−dipole interactions. Since adsorbates on metals are usually mobile, they spread out to form phases where the adsorbates are as far from each other as possible and dipole−dipole repulsion energy is minimized.[1−5]

On semiconductors, very electronegative adsorbates tend to form polar bonds. Since these bonds again act as dipoles, one would expect the same repulsive interactions as on metals. However, in several cases adsorbates are found to cluster (O_2/Si(001),[6−8] Cl/GaAs(110) [9]), indicating an attractive interaction. Although similar effects have been seen in theoretical treatments,[10] a simple underlying explanation for this behavior has yet to be suggested. The situation is also confused by the fact that, due to the localized, directional bonding, adsorbates on these surfaces are often immobile. The adsorbate distributions are therefore strongly influenced by kinetics as well as energetics.

Using scanning tunneling microscopy (STM), we have found that chlorine atoms form clusters at room temperature while chemisorbed on the GaAs(001)-*c*(8×2) surface. Cluster size distributions indicate that the clustering occurs through postdeposition adsorbate diffusion. This is consistent with other work, in which we found single Cl adsorbates to have an anomalously high mobility on this surface due to multiple accessible adsorption sites.[11] Since the clustering occurs due to a postdeposition process, it is clear that the Cl adsorbates experience an attractive interaction. They are not simply frozen into energetically unfavorable clusters due to kinetics.

The mutual repulsion of the adsorbate induced dipoles is much reduced by the fact that the Cl−Ga bonds are not normal to the surface. The tilt of the bonds also increases the interaction between the Cl atoms and charge transferred to second-neighbor Ga atoms. Together, these effects provide a simple, electrostatic explanation for the adsorbate attractive interaction. The surface structure resembles an ionic crystal, with attractive interactions between unit cells.

As well as being a model system for the clustering of charged adsorbates, dry etching of GaAs(001) with chlorine is an important technique for the semiconductor industry.[12,13] However, the details of the etch process remain poorly understood. For instance, unlike other reconstructions, the Ga-rich c(8×2) surface is *not* etched by thermal Cl_2 at room temperature; instead the chlorine saturates at monolayer coverage.[14] Theory and wet chemistry experiments with GaAs(111)[15,16] have suggested that this Cl saturated surface is passivated against the adsorption of other species, a result which we have verified using samples prepared in ultrahigh vacuum.[17] To understand how this passivated surface is formed, it is crucial to understand not only the adsorption of the Cl, but also it's behavior once adsorbed.

II. Experimental Section

Epi-ready GaAs(001) wafers (*n*-type, Si doped at $\sim 2 \times 10^{18}$/cm^3, miscut $<1°$) were initially regrown ex situ with molecular beam epitaxy to a thickness of ~500 nm and capped with a protective layer of As. In our ultrahigh vacuum system (base pressure $<10^{-10}$ Torr), the As cap was desorbed by heating the sample to 450 °C for several hours. Residual contamination was removed by sputtering the 540 °C sample with 500 eV Ar^+ ions. Low-energy electron diffraction was used to investigate the reconstruction symmetry prior to imaging with the Park Scientific STM. The images shown in this paper were obtained using a sample bias of −3.5 V and a tunneling current of 0.2 nA. With this bias, the electrons tunnel from the electronically filled states on the surface to the STM tip.

This preparation method results in a very well ordered *c*(8×2) reconstructed surface with roughly 1000 Å terraces, as shown in Figure 1a. The primary defect is a low density of clusters of excess As, which do not disturb the structure of the underlying

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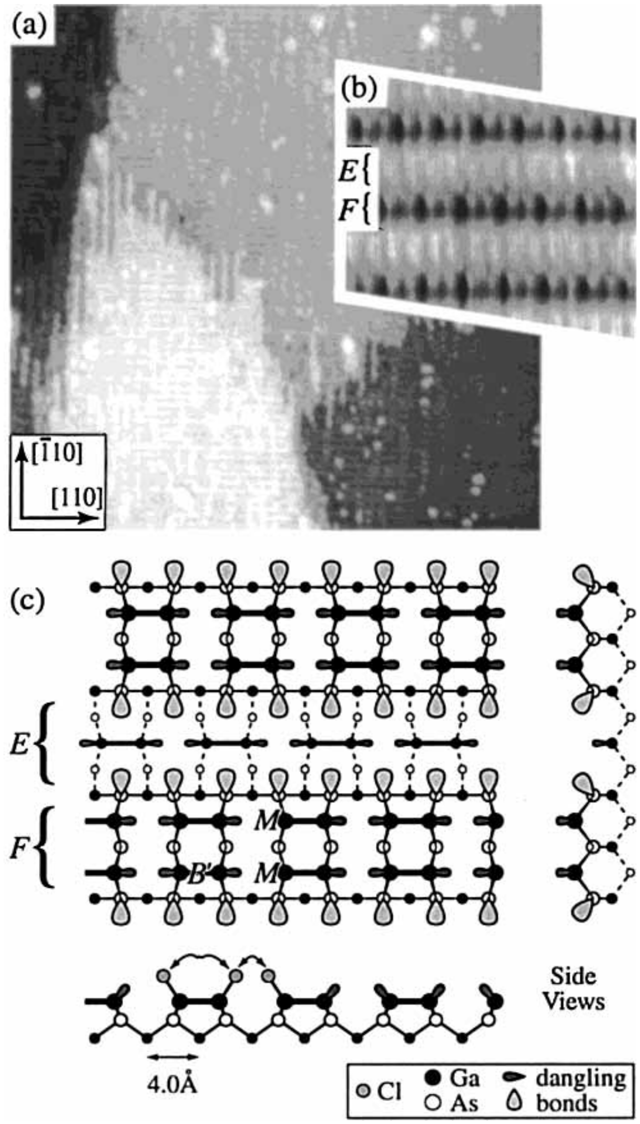

Figure 1. Clean Ga-rich GaAs(001)-$c(8\times2)$ surface: (a, b) filled state STM images of the surface, of size 1000 × 1100 Å^2 and 57 × 45 Å^2; (c) structure model for this surface. *M* labels the Cl adsorption sites, *B′* labels the slightly higher energy asymmetric bridge site. In the lower side view, the path for mobility of single, unclustered Cl atoms is indicated.

reconstruction. Our images of the clean surface agree with the most commonly suggested surface structure,[18,19] illustrated in Figure 1c. The surface consists of rows of parallel pairs of Ga dimers separated by trenches with filled As dangling bonds. Since As is more electronegative than Ga, As atoms appear far more prominent than Ga atoms in filled-state images. As noted by Xue et. al.,[20,21] in most cases the filled second-layer As atom dangling bonds actually appear higher than the first-layer Ga atoms. Thus the bright rows (*E* in Figure 1) are the second-layer As. In Figure 1b the dimerization of the first-layer Ga atoms can clearly be seen in the darker rows (*F*).

A pulsed supersonic molecular beam was used to dose the room temperature substrate with 0.11 eV Cl_2 molecules. The initial sticking coefficient under these conditions has been measured to be $S_0 = 64\%$.[22]

III. Previous Work

In other work, we have studied the adsorption site and behavior of Cl/GaAs(001)-$c(8\times2)$ at very low coverage, for which little adsorbate clustering occurs on the time scale of the experiment.[11] Although this paper does not rely on the results of that study, many of the conclusions are mutually supportive. We therefore include here a summary of those results.

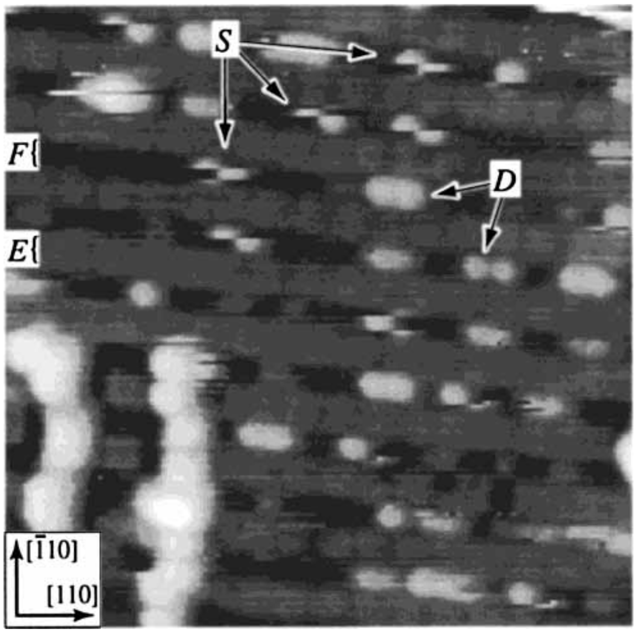

Figure 2. Horizontally scanned STM image of Cl adsorbed on GaAs-(001)-$c(8\times2)$ at a coverage 2.5% monolayer. Image size is 125 × 150 Å^3. Most Cl are single atoms (*S*), with a few pairs (*D*), *S* features show discontinuities due to motion on the time scale of the imaging process.

At coverages of a few percent of a monolayer, STM images show new features on the dark *F* rows of the $c(8\times2)$ reconstruction (see Figure 2). Most of these are single Cl atoms, labeled *S*, bonded to the empty dangling bonds of the Ga atoms to form a monochloride surface species (site *M* in Figure 1c). A few features, labeled *D*, are formed by two adsorbed Cl atoms, one on either side of a dimer pair. For both *S* and *D* features, the Cl atoms do not stay bonded to a single Ga atom. Each one hops along $[\bar{1}10]$ between two neighboring Ga atoms so rapidly ($\gtrsim 1$ kHz) that the STM cannot resolve the motion (see the two *M* sites in Figure 1c). The features therefore appear to be centered on the dark Ga rows.

The Cl atoms also show significant mobility along [110], parallel to the rows. If an atom moves while the STM is imaging it, the sudden change in position appears as a discontinuity in the image. The discontinuity will be parallel to the scanning direction, which is horizontal for the images in this paper. Almost all of the *S* features show such discontinuities. They always move along the *F* rows; since this is parallel to the scanning direction, the adsorbate position changes from line to line in the image. More detailed analysis finds that, on the order of once per second, each Cl hops 4.5 Å from one end of a Ga dimer to the other. An order of magnitude less often, the atoms make the shorter 3.5 Å hop between two Ga dimers. These long and short hops are illustrated in Figure 1c. The longer hops occur more frequently because they are facilitated by a low-energy intermediate bridge-bonded state (site *B′* in Figure 1c), where the Cl has inserted into the Ga dimer.

IV. Results

At higher coverages, the Cl adsorbates have been observed to cluster together. Figure 3a shows a surface with 4.3% monolayer of Cl, as calculated by counting features on the surface. The Cl remain centered in the dark *F* rows but are

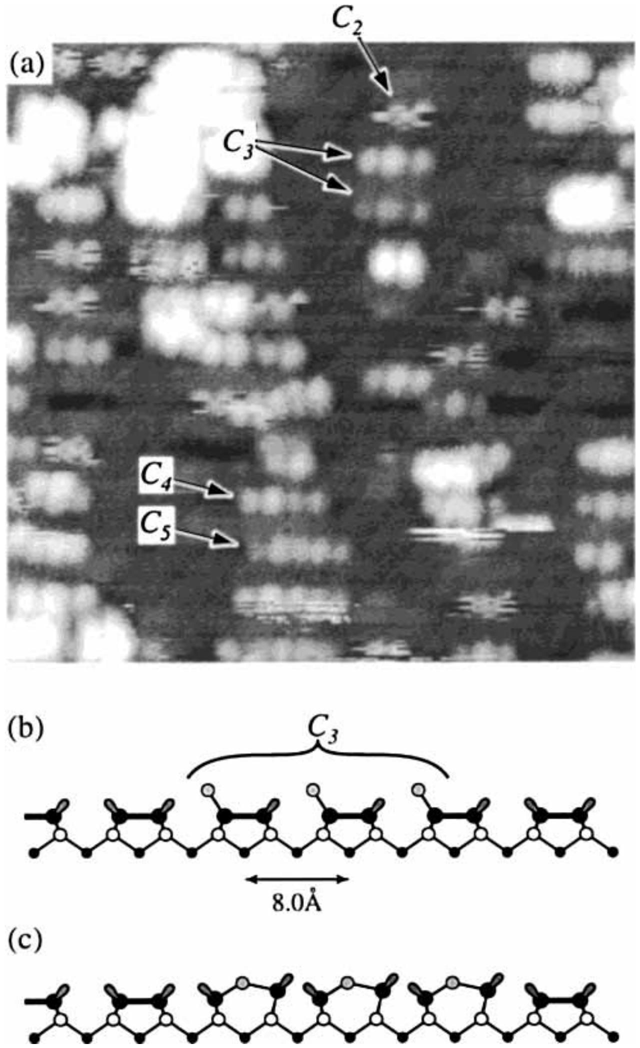

Figure 3. (a) A 250 × 200 Å^2 horizontally scanned STM image of Cl adsorbed on GaAs(002)-$c(8\times2)$ at a coverage of 4.3% monolayer. Cl has grouped into clusters (C_n) with 8 Å spacing between atoms. (b) Model structure for the Cl atom clusters based on the single atom monochloride structure. (c) Alternative structure, based on the asymmetric bridge site, which does not agree with C_2 mobility.

now clustered into linear groups parallel to the rows. The Cl atoms are spaced every 8.0 Å, or twice the lattice constant of the unreconstructed surface. If this were the densest allowed packing of adsorbates, this surface coverage would be equivalent to filling 34% of the adsorption sites. We label the clusters C_n, where n (the number of atoms in the cluster) was observed to range up to 6. Clusters of two atoms retain some mobility: the pair labeled C_2 moves back and forth 4.5 Å. In all observed cases, the motion was only between two positions and did not result in long-range cluster motion. The clusters were never observed to break up, and clusters of three or more atoms appear to be immobile.

The most natural site for an adsorbed halogen on this surface is as a monohalide species at the dangling bond of a Ga atom (site M in Figure 1c). This is similar to the site observed on other GaAs(001) reconstructions[23,24] and would agree with the adsorption site deduced for unclustered Cl atoms on this surface.[11] Figure 3b shows how three monochloride species would group to form a C_3 cluster. However, since Cl atoms have d-shell electrons, it is possible that the Cl might form a bridge-bonded configuration, either between Ga dimers or inserting into Ga dimers. Figure 3c illustrates the latter possibility. To distinguish between these options, recall that C_2 clusters are somewhat mobile, making long 4.5 Å hops back and forth between two sites. If the adsorbates were bridge-bonded, they should move in multiples of 4.0 Å, and by symmetry there could be no mechanism to restrict them to only two sites. Monochloride adsorbates could move from one end of a Ga dimer to the other, for which an apparent distance of 4.5 Å would be quite reasonable. Different energy barriers for intra- and interdimer motion could easily account for the tendency of a C_2 cluster to only visit two sites. Thus, although sufficient resolution was not obtained to directly image the Cl positions relative to the Ga atoms, the cluster structure in Figure 3b is well-justified.

There are several mechanisms which can, in general, result in adsorbate clustering. For instance, dissociative adsorption can result in pairs of adsorbates. However, it cannot account for the many clusters of size three observed here. Another route to clustering is induced reactivity for direct chemisorption, wherein an adsorbate raises the sticking probability at neighboring sites. However, for Cl/GaAs(001)-$c(8\times2)$ the initial sticking probability is so high that induced reactivity cannot have a large effect. A highly mobile physisorbed precursor state often results in clustering, but this mechanism is inconsistent with the many single chemisorbates observed at lower coverage (e.g., in Figure 2). Therefore the clustering is due to postdeposition diffusion, consistent with the anomalously high mobility which has been observed for individual Cl atoms.

To make this conclusion more quantitative, simple Monte Carlo computer simulations of several of these mechanisms were performed and compared with observations. A two-dimensional array represents an area on the surface: rows represent the F rows, and array elements represent dangling bond adsorption sites at roughly 4 Å intervals along the rows. To simulate simple random deposition, random sites are sequentially chosen, and an adsorbate is placed there unless a neighboring site is already filled. This enforces the 8 Å spacing observed in the clusters. To simulate induced reactivity, a chosen, open site is always filled if a next-nearest-neighbor site along the row is occupied, but otherwise the open site is only filled $S_0 = 64\%$ of the time. To simulate clustering by diffusion, after random deposition the program repeatedly chooses a random unclustered adsorbate and moves it 4 Å left or right along the row. All clusters are assumed to be immobile. The time span allowed for this diffusion is an adjustable parameter.

The results are presented in terms of the probability that a randomly chosen adsorbate will be in a cluster of size n. Meaningful error bars for the experimental observations are difficult to obtain because they depend on the image size, which varies widely. (The larger the image, the less the observed cluster distribution should deviate from the actual distribution.) It is much easier, and in this case sufficient, to simulate a specific experimental image. In this case the observed cluster size distribution is exact. Numerous simulations are run for the same surface area and adsorbate coverage as the experimental image, until standard deviations of the mean for the simulated probabilities are less than 1%. This leads to a simulated distribution of possible results which can be compared with the observed image.

Figure 4 compares the cluster distribution in Figure 2 with simulated results for clustering by both induced reactivity and diffusion. Results for several other images were similar. The boxes in the graph show plus and minus one standard deviation in the simulated distribution of possible results.

Because the initial sticking probability S_0 is so high, the results for induced reactivity are only slightly different from the results

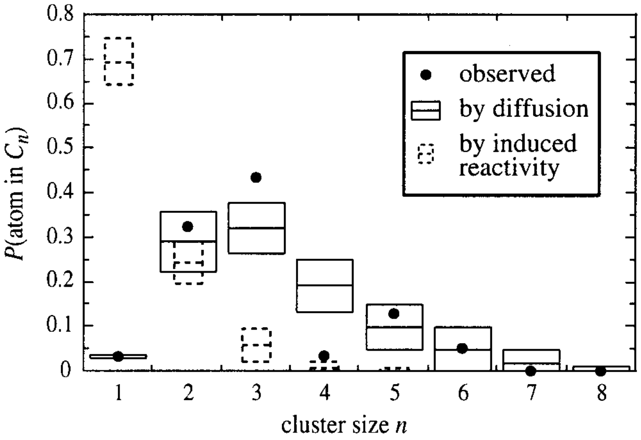

Figure 4. Graph of the probability that a given atom will be in a cluster of size *n*. Simulation results (boxes) show ±1 standard deviation in the random distribution of results.

for simple random deposition (not shown). Both of these cases are very different from the observed distribution, with single adsorbates dominating.

For the simulations of clustering by diffusion, the diffusion was allowed to proceed until the simulated number of unclustered atoms was equal to the observed number. The resulting simulated distribution matches the experimental data very well. In particular, it produces a fair number of clusters in the size range 4−6. Together, these simulations support the conclusion that diffusion is the clustering mechanism.

V. Discussion

Since the clustering is a result of adsorbate diffusion, it must be energetically favorable, rather than frozen in by kinetic barriers. There must be an attractive interaction between the adsorbed Cl atoms. This is contrary to what would be expected on the basis of the simplest electrostatic argument. The Cl−Ga bond, with an electronegativity difference of $3.16-1.81 = 1.35$, is expected to have 38% ionic character.[25] The similarly charged adsorbates should have repulsive, not attractive, interactions.

Electrostatic arguments have been used successfully to analyze the energetics of reconstructions of the clean surface.[26] To do this carefully, the atomic geometry and the charge distribution must be considered. For instance, the simple argument above assumes that the induced dipoles are normal to the surface. But the Cl−Ga bonds will clearly not be normal to the surface. Indeed, at the other extreme, dipoles placed end to end parallel to the surface would be attractive, forming a one-dimensional ionic crystal.

In order to have numerical values to pursue this reasoning further, ab initio calculations were performed to determine the preferred geometry of small clusters simulating the GaAs(001)-$c(8\times2)$ surface plus a single adsorbed Cl atom. The GAUSSIAN94 computer program was used to minimize the cluster energy under the effective core potential (ECP) scheme of the Hartree−Fock approximation. No higher-order corrections (such as Møller−Plesset perturbation) were used. The LanL2MB basis sets and ECPs were used. The criteria for full relaxation were the program's defaults. For more details concerning the calculation, refer to ref 27.

Figure 5a shows the results for a $Ga_{20}As_{20}H_{32}Cl_1$ cluster that simulates two parallel Ga dimers of the $c(8 \times 2)$ surface. Hydrogen atoms terminate bonds that would be in the bulk crystal. The adsorption of the Cl atom has hardly disturbed the Ga dimer of length 2.87 Å. The Cl−Ga bond has a length of 2.38 Å and is tilted from the surface normal by 40° toward [110]. Mulliken population analysis for a similar cluster with no Cl atom indicates a charge of $+0.12e$ on the dimerized Ga atoms of the clean surface. For the cluster in Figure 5a the Cl atom has a charge of $-0.50\ e$, the neighboring Ga atom (Ga_A) gains a charge of $+0.34\ e$ relative to the clean surface, and the next-neighbor Ga atom (Ga_B) gains a charge of $+0.05\ e$. Other atoms in the cluster change charge by $<0.02\ e$.

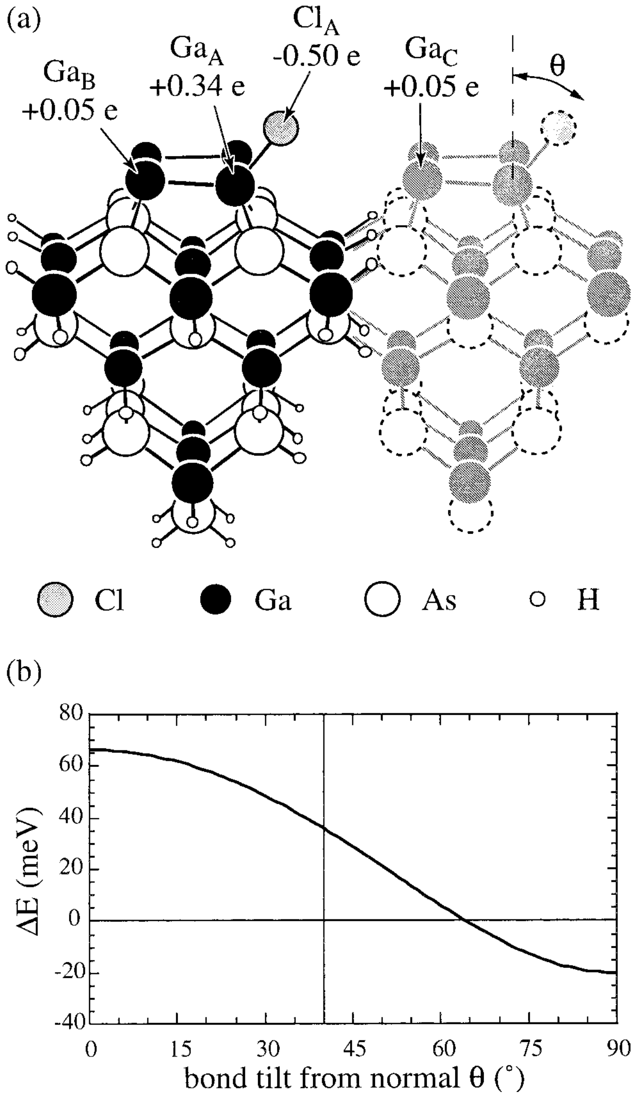

Figure 5. (a) Optimized geometry cluster model for Cl on GaAs(001)-$c(8\times2)$. The dark left half is the actual cluster, viewed from 15° out of the surface plane. In the grey right half the cluster (without terminating H atoms) is duplicated to continue the surface, in order to consider clustering energetics. (b) Graph of the interaction energy between two neighboring Cl−Ga dipoles as a function of their angle from normal. This does not consider the effects of the second neighbor Ga atoms.

Using these charges and atom positions, we now calculate the electrostatic interaction energy between two adsorbed Cl atoms at the clustering distance of 8.0 Å, as shown by the second grayed cluster in Figure 5a. The atoms are approximated as point charges. Note that to calculate the electrostatic interaction between two adsorption sites, we must only consider the extra charge induced on the Ga atoms. Any interaction involving the clean surface Ga charge will be present whether the Cl atoms are there or not.

First we consider only those atoms with large induced charge: the Cl atoms and the nearest Ga atoms. The dipole−dipole repulsion is significantly reduced by the fact that the Cl−

Ga bond is not normal to the surface. Using the calculated charges and bond lengths, Figure 5b shows how the interaction energy of two Cl−Ga dipoles depends on the bond tilt angle. At 40°, the tilt predicted by the cluster calculation, the repulsion is reduced by almost 50% to 36 meV.

The interaction energy between any pair of the highly charged atoms (Ga_A and Cl_A) on neighboring sites is on the order of 500 meV. However, they tend to cancel out, leading to a relatively small net interaction. As a consequence, smaller, secondary charging can have a significant effect. Most importantly, in Figure 5a the interaction of the $+0.05\ e$ charged Ga_C with Cl_A is attractive. Totaling all interactions of these next-neighbor Ga atoms (for example, Ga_C-Ga_A repulsion), their net effect is an energy reduction of −43 meV. Combining this with the Ga_A-Cl_A dipole−dipole repulsion energy, we find that adsorption sites should indeed cluster, with a binding energy of $36-43$ meV $= -7$ meV.

Electrostatic calculations for point-charge atoms cannot be expected to provide very exact energies. Indeed, since the clusters were never observed to break apart, the actual cluster binding energy should have a magnitude $> kT = 25$ meV. Broadly, however, this analysis clearly identifies two major factors contributing to the clustering of charged Cl adsorbates on the GaAs(001)-*c*(8×2) surface. The naive repelling-dipole model breaks down, but considering more information about atom placement and charging can restore electrostatic arguments to a useful position.

VI. Conclusion

When Cl adsorbs on Ga-rich GaAs(001)-*c*(8×2), there is significant charge transfer, resulting in adsorbate induced dipoles. Naively, this would lead to dipole−dipole repulsion; nevertheless, at moderate coverages the adsorbates tend to cluster together. The anomalously high one-dimensional mobility of Cl on this surface makes it an ideal model system for this kind of behavior. Since the clustering happens through diffusion (as corroborated by the cluster size distribution), we can be certain that the clustering is not frozen in by kinetic barriers, but is instead driven by energetics. The Cl adsorbates feel a net attractive force.

The attraction can nevertheless be understood by considering only electrostatics. We find two general effects. First, considering only the Cl adsorbate and the substrate Ga to which it is directly bound, the induced dipoles are tilted from the surface normal. As a result the surface structure more closely resembles that of an ionic crystal, and dipole−dipole repulsion is significantly reduced. In other systems, this may even result in an attractive interaction. For instance, this might occur for oxygen, which tends to adsorb low into surfaces in order to form two bonds.[28,29]

Second, the adsorbate's next-nearest neighbor is placed far from the adsorbate, in the same direction as the nearest neighbor. Therefore, this next-nearest neighbor can get close to a second adsorbate, and their interaction can have an important effect. For example, in Figure 5a Ga_C can get close to Cl_A without getting too close to Cl_A's bonding neighbors. We can think of the next-nearest neighbor as effectively extending the adsorbate induced dipole, significantly increasing its tilt from the surface normal.

In comparing this system to charged adsorbates on metals, which generally do not cluster, the most important difference is the directional bonding of the semiconductor substrates. This directional bonding is what allows the adsorbate bond to be tilted. It is also necessary for the surface reconstructions which have second-nearest neighbors asymmetrically distributed. This second effect, in particular, is likely to be most important on heterogeneous semiconductors, which tend to have complex surface reconstructions.

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