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Local dimer-adatom stacking fault structures from 3×3 to 13×13 along Si(111)-7×7 domain boundaries

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Regular domain boundaries (RDB's) on the Si(111)-7×7 surface are investigated both theoretically and experimentally. It is found that in most cases the defects in the RDB are accompanied by dimer-adatom stacking fault subunits or units (DAS cores, from 3×3 to 13×13) which span the RDB as matching bridges and stabilizers. The RDB's with DAS cores directly reveal dynamic messages of DAS reconstruction. Total energies of the larger DAS systems and interactions between some local configurations, e.g., dimers and adatoms are calculated using the empirical building block method which includes the charge-transfer effect and the dimer-adatom interaction. This study also indicates that the larger DAS members have lower energies than conventionally expected. [S0163-1829(98)05244-8]

I. INTRODUCTION

There are several reconstructions on the Si(111) surface and they have been intensively studied for nearly half a century. Among them the series of dimer-adatom stacking fault (DAS) structures, i.e., 3×3, 5×5, 7×7, 9×9 (Refs. 1–10) and even 11×11, 13×13,[11] always have a general appeal in surface science. This is because of the strong motivation to discover the driving force for such complex yet stable reconstructions. Early studies often divided these large systems into smaller building blocks to analyze the energetics[4,5] and the origin of the electronic states[6] under the zeroth approximation. Some important properties, e.g., the role of dimer row[4] and the stability of 7×7,[5] were disclosed. The first *ab initio* calculation on Ge(111)-3×3 disclosed the role of adatoms which had been underestimated by Vanderbilt.[4] So far, fully *ab initio* calculations can only be achieved on the first three of the DAS series[8] because a colossal number of atoms in larger ones retard any attempt of this kind. The extremely accurate *ab initio* method also suffers from another inconvenience, i.e., apparent dynamic messages cannot be directly drawn from the result. Obviously, one cannot expect all the physics underlying the reconstructing process of such complex systems to be exposed in the perfect lattice. As it is known, defects are always more informative in that they can be considered as being frozen at a series of metastable states before the formation of the perfect lattice. Fortunately, there are several types of well-constructed defects on Si(111)-7×7 surface which can give definite messages.

Both qualitative and full *ab initio* studies show that 7×7 reconstruction is the most energetically favorable structure. Hence, the Si(111)-7×7 surface can be easily obtained in large area with the sample annealed slowly enough under careful control. This does not imply that there exist no noticeable defects in this case. In fact, the surface is always divided into domains by some local defects which can be clearly observed with a scanning tunneling microscope (STM). The groups of the defects are thus referred to as domain boundaries.[12,13,10,14,15] Although the domain boundaries are sparse on the surface, they carry more dynamic messages in that their structures are more complicated and vary a lot. However, in most cases, the defects on the domain boundaries have irregular structures, so the energetic analysis of their formation is quite difficult. Only the well-defined defects in the atomic scale have the value for investigation. Hadley and Tears[13] observed a regular structure which is assumed to be initiated by some defects during the cooling process and to propagate with the growing of 7×7 reconstruction. Recently Gu *et al.*[16] reported a series of regular domain boundaries (RDB) and gave their atomic structures roughly. An important characteristic of all the RDB's they observed can be thought to form in the same way, i.e., relative shifting between two adjacent parts of the perfect lattice. The outline and direction of the RDB is mainly determined by the shift except that the details of the atomic structure are modified by local adjustment of the atomic positions within the defects. Itoh *et al.*[17] classified the RDB's in a systemic scheme by introducing a phase shift vector. In this way, a complete study on RDB's become possible and most of the RDB's observed in their experiment can be included in the theoretical categories.

In this study we find most of the RDB's have DAS cores (i.e., the defects along the RDB's are accompanied by local DAS reconstructions) which serve as matching bridges and stabilizers. These types of RDB's, to our knowledge, have not been studied energetically as a whole series. The materials of this paper are arranged as follows. In Sec. II, experimental results are presented. Instead of doing simply structural analysis we focus on the variations of the structures of the local defects to extract dynamic messages and try to find out the driving force for the formation of the structures. Based on the spirits discussed in the experiment, we present in Sec. III an empirical method for energetic calculation on the DAS reconstruction series. Finally, the main points of this study are summarized in Sec. IV.

II. ANALYSIS OF THE EXPERIMENTAL RESULTS

Actually, several types of RDB's with 3×3, 5×5, and 9×9 cores have been observed, respectively, by other authors except that they did not consider them as a whole se-

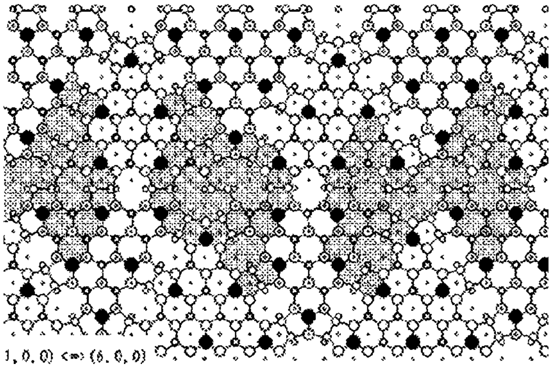

FIG. 1. Structural model of a section of RDB with 7×7 cores.

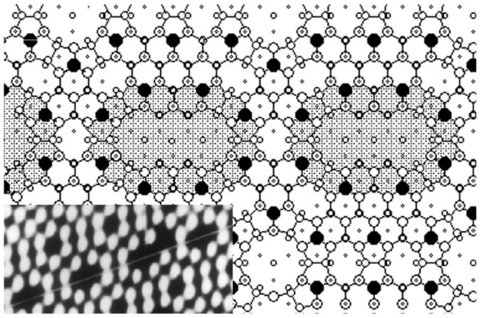

FIG. 2. Structure model for a section of RDB with 5×5 cores. Inset: STM image of empty states.

ries. Since the surface studied here is 7×7, we regard the RDB without any of the above local reconstructions as RDB's with 7×7 cores. In our experiment, a new RDB with 13×13 cores is observed, therefore the series of RDB's on the Si(111)-7×7 surface now covers the local DAS reconstructions from 3×3 to 13×13 except that 11×11 has not been spotted. The experiment in this study is the same as that of Ref. 16.

The RDB's with 7×7 cores appear most frequently in our experiment. This is easily understood since 7×7 is the most energetically favorable in the DAS series. Among them, there is a very interesting RDB (see Fig. 1 for the new structural model given by us) that should be mentioned. Itoh *et al.*[17] observed this RDB but gave a structural model with too much dangling bonds. Gu *et al.*[16] noted that a typical defect is formed from the 7×7 subunit (faulted or unfaulted) by missing an adatom on the bottom line and the other two adatoms adjust their positions following the dimer row along the RDB. This is an apparent manifestation of the interaction between the dimer and the adatom.[7] That is why we will include the dimer-adatom interaction in our calculation in Sec. III. Gu *et al.* also gave a complicated yet unconvincing explanation on the alternative appearance of the typical defects on the two sides of the RDB. In our model, the continuous dimer row along the RDB directly explains the alternative appearance of the defects. Energetically, when the rings around the corner holes are broken to open to the outside atoms, a continuous dimer row is preferable along the RDB so that a firmer backbone is constructed. As a result of interaction between the adatoms and the dimers, the defects have to be arranged by the dimer row. Since the period of the dimer row is $2a_0$ and that of 7×7 subunit is $7a_0$, the period of the RDB is naturally the products of them, i.e., $14a_0$ ($a_0 = 3.85$ Å is the length of the translational vector of the ideal 1×1 surface).

Several RDB's with defected 9×9 subunits often appear in our experiments. For example, the earliest reported RDB (Ref. 13) and the one reported by Itoh *et al.* (see Fig. 9 in Ref. 17). All these RDB's are clearly built indicating the quite lower energy of 9×9 reconstruction in the whole series.

Figure 2 shows a RDB with a core of full 5×5 unit cells. This RDB seems less stable than that with cores of unfaulted 5×5 subunits reported by Gu *et al.* (see Fig. 5 in Ref. 16). This is because the large holes along the RDB screen off dimers therefore the backbone is not so firm. This RDB is an example of the RDB's that are beyond the scope of Itoh's classification system.[17]

The most complex RDB we have found is that with 13×13 subunits (unfaulted half, see Fig. 3). Basically it is a regular structure with the period of $14a_0$ except that the adatom missing appears sometimes in the 13×13 subunits. Note that if the dimers bordering the defects specified by the ellipse disintegrate then a large strip of 2×2 reconstruction with three rows of adatoms will be formed. And also note the strip with width of $6a_0$ can be filled by another local reconstruction, i.e., 3×3 unit cells. However, all these possible structures give way to the 13×13 subunits. This implies that the larger DAS members may have lower energies than conventionally expected.

A RDB with 3×3 cores has been shown as Fig. 6 in Ref. 16. Here we present a more precise structural model for it (Fig. 4). In the present model, only a subunit of 3×3 is constructed with adatom **z** in it, while no 3×3 subunit is

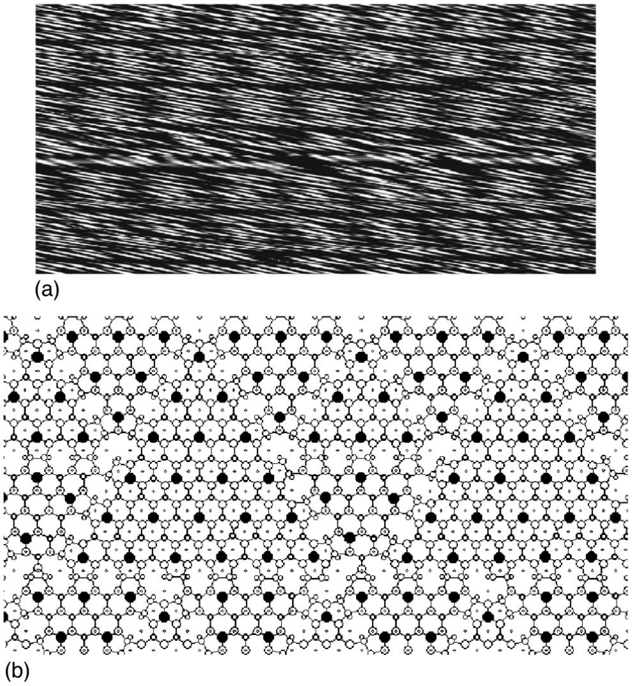

FIG. 3. A section of RDB with 13×13 cores: (a) STM image of empty states. The defect specified by the circle is the same as in Fig. 1, while that specified by the ellipse is a new one. The triangles specify the 13×13 subunits. (b) Structure model.

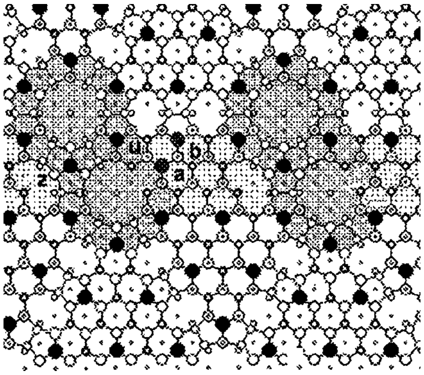

FIG. 4. Structure model for the RDB with 3×3 cores. Between the two corner holes in each pair there exists a subunit of 3×3 with adatom **z**.

formed around adatom **u**. This is because adatom **u** is a little lower (in STM image, a little darker) than adatom **z**. The height difference between these two adatoms vividly shows that in 3×3 reconstruction the condensation of the corner holes make the dimers hold up each other to prevent the triangles of the backbond atoms beneath the adatoms from expensing.[8] This is important for the evaluation of spring constants s_i in the calculation (Sec. III). The overly piled up adatom **a** and **b** (Fig. 4) account for the large bright dots (in the STM image) near adatom **z**.

So far we have not found the RDB with 11×11 cores. For the DAS members larger than 7×7, only the unfaulted subunits have been observed to appear in RDB's. This is because the stacking fault is the only passive factor for DAS reconstruction among its three characteristic configurations (i.e., dimer row, adatom, and stacking fault). Since defects are permitted in the RDB's, the larger cores will naturally throw off the heavy blocks of the faulted subunits. Because the unit cells of DAS structures are quite large and they are confined by the dimer rows, the interaction between the DAS cores and the circumstance is weak. Consequently, we assume the stability of the RDB's reflects the surface energies of the corresponding DAS members in their perfect reconstructions. From the STM images and the chance they are observed we can roughly rank the energy order (at least for the unfaulted halves) from low to high as 7×7, 9×9, 5×5, 13×13, 3×3. In the following part, we will present some calculation on the energies of the DAS series.

III. CALCULATION OF THE TOTAL ENERGIES AND LOCAL INTERACTIONS FOR THE DAS RECONSTRUCTION SERIES

There are mainly three factors which contribute to the surface energies of DAS reconstructions. First, the formation of dimer rows is an important driving force for the reconstructions.[4] The dimer rows reduce dangling bonds on the surface with much less strain introduced than the adatoms do. Without the dimers, the energy lowered from the reduction of dangling bonds by the adatoms will almost be canceled by the strain energy introduced by the adatoms themselves. However, the strain energy introduced by an adatom may be partly counteracted by the dimer nearby, which results in interaction between the adatom and the dimer. This accounts for the fact that adatoms in both the perfect DAS reconstruction and the defects in the domain boundaries will always prefer to be adjacent to the dimers. So the interaction in the adatom-dimer pairs is the second factor that stabilizes the DAS structures. The third factor is the charge transfer from the dangling bonds on the adatoms to that on the rest atoms. Such a charge-transfer effect is caused by the difference between the bonding environments around the adatoms and the rest atoms. That is, the stressed bonds around the adatom makes the local energy levels near the adatom higher than that around the rest atom whose bonds are less stressed. Charge transfer from the adatom to the rest atom therefore lowers the surface energy. However, charge transfer will release the stress of the bonds around the adatoms while raising the stress of the bonds around the rest atoms.[8] Another effect of charge transfer is to cause polarization which will also raise the surface energy. The charge transfer saturates at the equilibrium point of these opposite effects.

Although the DAS series have similar atomic configurations, the density of certain kinds of local configurations, e.g., dimers, adatoms, and rest atoms, in the unit cell is not the same for all the reconstructions.[5] The competition and balance between these local configurations and their interaction results in different energies of DAS members. For the smallest DAS reconstruction, i.e., 3×3, the strain energy caused by the adatoms and the dimers is confined in a so small area that its energy per unit area is raised as is directly shown in the RDB. With the unit cell getting larger from 5×5 to 7×7, the system relaxes considerably (i.e., the strain diffuses to larger area) hence the energy per unit area is lowered. In the meantime, there is an increase in the ratio of rest atoms to the adatoms as the unit cell becomes larger,[5] therefore charge transfer from the dangling bonds of the adatoms to that of the rest atoms increases to lower the surface energy. However, with the unit cell becoming further larger (or rather the ratio of rest atoms to adatoms further higher), the charge transfer will saturate early before all electrons on the dangling bonds of the adatoms are transferred out. On the other hand, adatoms without adjacent dimers (we refer to these adatoms as isolated adatoms) which appear first in 9×9 considerably raise the energies of larger DAS members. All these considerations constitute the basis of the following calculation.

The idea that the total energy of DAS structures can be roughly calculated by constructing building blocks for typical local configurations has been implied in several works.[4–6] It seems to us the previous building block methods suffer from two drawbacks. First, the energies of the building blocks have to be precalculated using other methods (e.g., empirical method is used in Ref. 5). Second, as a zeroth-order approximation, they did not include such effects as dimer-adatom interaction and charge transfer which are important for stabilizing the DAS structures. Here we will select a new set of building blocks and refine this method to the first order by including some interaction terms. In our method, the energy blocks are basic parameters which are determined in the same time when the whole problem is solved by fitting to the first-principles results. We divide the subunit of a DAS structure into three types of adatom-specific building blocks (rhombus in Fig. 5): the elementary

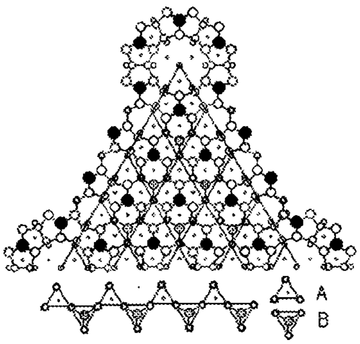

FIG. 5. Building blocks in the unfaulted Si(111)-9×9 subunit. The block in each rhombi is an adatom-specific building block; the triangle pairs in the bottom denote the rest atom blocks with A negative and B positive. The shaded circles denote the rest atoms.

block (E_i) corresponding to the isolated adatoms and two derivative blocks, i.e., the center adatom block E_c, and the corner adatom block E_h

$$E_c=E_i+\Delta, \quad E_h=E_i+2\Delta+\delta. \tag{1}$$

Here Δ is the perturbation of the dimer on the adatom block, it consists of the strain of the dimer and the adatom-dimer interaction I_{ad}, δ denotes the interaction between two adjacent dimers near the corner hole. Generally, the local interaction, e.g., I_{ad} are not the same for all DAS members. However, the constant perturbation only accounts for one part of the corresponding interaction, while the other part that depends on the individualities of the DAS members will be included in the charge-transfer term. The dangling bond in the corner hole is described by another elementary block h_0. The numbers of the adatom-specific building blocks corresponding to the corner adatoms, center adatoms, and the isolated adatoms in each $(2n+1)\times(2n+1)$ unit cell are

$$N_h=6, \quad N_c=6(n-2), \quad N_i=(n-2)(n-3), \tag{2}$$

respectively.

If the total energy of the $(2n+1)\times(2n+1)$ DAS system is obtained by summing up all these building blocks, n type-A blocks (see Fig. 5 where $n=4$) are undercounted and n type-B blocks are overcounted in each subunit. Consequently, the last elementary block is introduced as the rest atom block E_r which is the energy of the (1×1) triangular subunit with a rest atom (type-B block) subtracted by the energy of the other (1×1) subunit without any rest atom (type-A block).

The stacking fault is considered in the same way as Qian and Chadi.[5] That is, the energy shift caused by stacking fault in a $(2n+1)\times(2n+1)$ unit cell is

$$E_f=0.04\frac{(2n+1)^2}{2}=0.02(2n+1)^2. \tag{3}$$

The interaction between the dangling bonds on adatoms and rest atoms is included by a charge-transfer term. The charge-transfer term is defined as the energy contributed by the charge transfer relative to the state with strict charge neutrality at any site (supposing the occupation number at each site is the same q_0):

$$E_T=\sum_{i=1}^{d}\left[-n_i(\epsilon_i q_i+s_i q_i)+n_i(Uq_i^2)\right], \tag{4}$$

where d is the number of typical dangling bonds with n_i members in each type, q_i is the net charge (occupation relative to q_0) on the atom with the dangling bond i, ϵ_i is the energy level of the dangling bond state, $s_i q_i$ is the strain energy reduction introduced from charge transfer,[8] and Uq_i^2 is the Hubbard-like on-site energy with $U=1.0$ eV.[18]

The following points should be stated about s_i: (a) We have made an assumption in Eq. (4) that the reduction in strain energy introduced by the charge transfer from the ith dangling bond to other dangling bonds is linearly scaled by the factor s_i. This approximation works because the charge-transfer volume is always small in the perfect lattice. For an adatom dangling bond with positive net charge volume, the strain energy in its vicinity is reduced by the charge transfer; the case is reversed for a rest atom.[8] (b) The s_i for corner adatoms, center adatoms, and isolated adatoms are not the same. For the center adatom which has one neighboring dimer, the charge transfer from its dangling bonds leads to lowering of the backbonds atoms hence makes the bond of the dimer stronger.[8] That is, more charge transfer is energetically favored by the adatom-dimer interaction. For a corner adatom, the two adjacent dimers beside it hold up each other to prevent the lowering of the backbonds atoms. That is, charge transfer is not favored by the dimer-dimer interaction. Finally, the isolated adatom without a neighboring dimer will not give out much charge. (c) The s_i for corner adatoms in smaller DAS members 3×3 and 5×5 cannot be the same values as larger ones. As it is shown in the domain boundary, the condensation of dimers prevent the triangles of the backbond atoms beneath the adatoms from expensing because the adjacent dimers hold up each other. We choose the same s for corner adatoms in the members from 7×7 up to 13×13, while that of (corner) adatoms in 5×5 is scaled by 1/3 and that in 3×3 is set to zero. Otherwise, no satisfactory result can be obtained.

The total energy of the $(2n+1)\times(2n+1)$ unit cell is

$$E_n=h_0+N_hE_h+N_cE_c+N_iE_i-2nE_r+E_T+E_f \tag{5a}$$

$$=h+n(n+1)E_i+2nD+E_T+E_f, \tag{5b}$$

where

$$h=h_0+6\delta, \quad D=-E_r+3\Delta. \tag{6}$$

$2nE_r$ in Eq. (5a) is the double counting term which should be deducted from the sum of the adatom-specific building

TABLE I. Local states and charges (only for 7×7) on the dangling bonds. H, R, Ai, Ac, and Ah denote the dangling bonds on the corner hole atom, rest atoms, dimer-free adatoms, center adatoms, and corner adatoms.

	H	R	Ai	Ac	Ah
ϵ (eV)[a]	−0.8	−0.8	−0.2	−0.2	−0.2
s (V)	0.1	0.1	0.2	1.1	0.6
q(e)	−0.379	−0.429		0.371	0.121

[a] All the values in this line are chosen according to Ref. 9.

TABLE II. Total energies and charge-transfer terms of several reconstructions on Si(111) surface (per 1×1 area).

Recst	$T_4-(2\times2)$	3×3	5×5	7×7	9×9	11×11	13×13
E_T (meV)	-15.0	-2.9	-8.9	-44.1	-50.6	-52.5	-52.3
E (eV)	1.279[a]	1.196[a]	1.168[a]	1.153[a]	1.164[a]	1.176[a]	1.186[a]
E (eV)	1.273[b]	1.196[c]	1.168[c]	1.153[c]	1.157[d]		

[a] Present work.
[b] Reference 19.
[c] Reference 8.
[d] Reference 11.

blocks. This term represents the reduction of dangling bonds as a result of the formation of dimers. Although Eq. (2) applies only for $n\geqslant2$, it can be tested that Eq. (5b) is true for all the DAS members.

Basically, ϵ_i are chosen to be $-0.2+E_F$ for the dangling bonds on adatoms and $-0.8+E_F$ for those on rest atoms and the corner hole atom,[9] where the Fermi level E_F can be set to zero because only the relative energies of the levels affect the charge-transfer term. These values for ϵ_i are transferable within the whole series with good accuracy.[6] On the otherhand, s_i's are adjusted to reproduce E_i as close to the energy of 2×2 as possible and also to reproduce reasonable net charge on the dangling bonds of 7×7. Once ϵ_i's and s_i's are chosen (Table I), the charge-transfer term can be calculated by minimizing Eq. (4) with respect to q_i under the constraint of charge neutrality $\Sigma_{i=1}^{d}n_iq_i=0$. Consequently, the other three parameters h, E_i, and D are determined as $h=2.604$ eV, $E_i=5.177$ eV, and $D=-1.173$ eV from the *ab initio* result for 3×3, 5×5, and 7×7.[8] With these parameters the energies of 9×9, 11×11, and 13×13 are calculated following Eq. (5b) and shown in Table II as compared to the smaller DAS structures.

We can see that the energy of 9×9 is indeed a little lower than that of 5×5 which is consistent with that estimated by Yang and Williams in their experiment.[11] The fact that the energy of 13×13 is a little lower than 3×3 is surprising yet consistent with our experimental results discussed above. That larger reconstructions are less often observed in experiments than the smaller ones are not because the former ones are less energetically favorable but because they have higher density of atoms while no sufficient atoms can be provided in ordinary conditions.[11] It is also shown that even the surface energy of 3×3 is lower than other reconstructions such as $T_4-(\sqrt{3}\times\sqrt{3})$ and $T_4-(2\times2)$.[19] That is why DAS local reconstructions often appear on RDB's. From the second line of Table II we can see the charge-transfer terms saturate at 9×9 and remain quite low at 13×13.

Local interactions can be easily deduced from the results. Since there is a dangling bond on each corner hole atom and on each rest atom, we assume $h_0=E_r=1.343$ eV, which is the energy of relaxed 1×1 surface per unit cell.[19] The interaction between two adjacent dimers is obtained following Eq. (6): $\delta=0.210$ eV, while $\Delta=0.057$ eV. Obviously we have $\Delta=D_{\mathrm{strain}}/2+I_{\mathrm{ad}}$, where $D_{\mathrm{strain}}=0.53$ eV is the strain energy per dimer.[5] The interaction between the dimer and its adjacent adatom I_{ad} is -0.208 eV. As we have stated, this interaction value is the constant part that does not include the dimer-adatom interaction part that is caused by charge transfer. Since there is little charge transfer in 3×3, this value can be considered as the full interaction for one fold of adatom-dimer coordination in 3×3. To compare with our $I_{\mathrm{ad}}=-0.208$ for Si, we estimate the corresponding value for Ge on the basis of Payne's results.

Employing the *ab initio* method, Payne obtained the Ge(111) surface energies of ideal (1×1), fully relaxed (1×1), T_4-(2×2), DAS-(3×3), and adatoms-free (3×3) [i.e., adatoms are desorpted from DAS-(3×3)] as $E_{(1\times1)\mathrm{idl}}=1.22$ eV, $E_{(1\times1)\mathrm{rlx}}=1.15$ eV, $E_{(2\times2)}=4.16$ eV, $E_{\mathrm{DAS}(3\times3)}=7.95$ eV, and $E_{(3\times3)}=10.06$ eV. First, the contribution of the isolated adatom to the surface energy is

$$E_{(2\times2)}-4E_{(1\times1)\mathrm{idl}}\leqslant e_{\mathrm{is}}\leqslant E_{(2\times2)}-4E_{(1\times1)\mathrm{rlx}}. \tag{7}$$

Substitute the corresponding values, we get $-0.72\ \mathrm{eV}\leqslant e_{\mathrm{is}}\leqslant-0.44$ eV. Second, when the DAS-(3×3) is constructed by depositing adatoms to the adatom-free (3×3), the lowering in surface energy is contributed by both the adatoms and the dimer-adatom interaction. Notice that there are two adatoms each with threefold dimer-adatom interactions in each DAS-(3×3) unit cell, and we have

$$I_{\mathrm{ad(Ge)}}=\frac{1}{6}[E_{\mathrm{DAS}(3\times3)}-E_{(3\times3)}-2e_{\mathrm{is}}]. \tag{8}$$

Finally, the dimer-adatom interaction energy for germanium DAS reconstruction is obtained $-0.205\ \mathrm{eV}\leqslant I_{\mathrm{ad(Ge)}}\leqslant-0.111$ eV. Now it is seen that our result of dimer-adatom interaction for Si is quite reasonable.

IV. CONCLUSION

We have presented an energetic investigation on the serial RDB's with local DAS reconstructions. The following points should be reviewed. (1) Local DAS reconstructions play an important role in the formation of RDB's for two reasons: (a) It is a lattice matching condition for them to appear along RDB's; (b) The DAS structures up to 13×13 are energetically more favorable than other local reconstruction such as T_4-(2×2), $\sqrt{3}\times\sqrt{3}$ *et al.* (2) Dynamic messages on the DAS series are directly revealed by the RDB's with DAS cores: (a) The order of DAS members in energy from low to high is reflected from the stability of the RDB's with the corresponding cores; (b) The role of dimers, adatoms, and-stacking fault can be apparently seen from typical defects. (3) By roughly including the charge-transfer effect, the empirical building block method yields not only the correct order in surface energies of the DAS members but also a reasonable energy value for the dimer-adatom interaction.

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[19] Northrup gave the surface energies for unrelaxed (1×1), relaxed (1×1), T_4-(2×2), and T_4-$(\sqrt{3}\times\sqrt{3})$ as 1.63, 1.46, 1.39, and 1.35 eV per (1×1) area (see Ref. 6). However, Needles obtained the surface energy for unrelaxed (1×1) as 1.513 eV in a similar condition to that of the calculation for the first three DAS members in Ref. 8. To keep consistent, we shift Northrup's values down by 0.117 eV to obtain the surface energies for unrelaxed (1×1), relaxed (1×1), (2×2), and $(\sqrt{3}\times\sqrt{3})$ as 1.513, 1.343, 1.273, and 1.233 eV.