~001! surface having the same projected ~001! area. Because the concentration of H is different in each phase, and because steps can introduce a local change of the H density with respect to the flat surface, both the surface and step formation energies are functions of the H chemical potential m_{H}. In Fig. 1, the highest value of m_{H} ~taken here as zero! is that at which H extracts without energy cost Si atoms from the surface, forming the SiH_4 molecules.[21]

III. FLAT SURFACE

Figure 1 shows schematically calculated surface formation energies of clean Si~001! @Fig. 1~a!# and hydrogenated Si~001! @Fig. 1~b!#

formation energy of $S^{*}_{\perp} 1 S^{*}_{\perp}$ to estimate $l\ (S^{*}_{\perp}) 5$ $2\,0.27\ \mathrm{eV}/a$. The reasons for a negative formation energy of $S^{*}_{\perp}$ are twofold: ~i! Steric energy reductions at the step edge: One may write the step energy l as $l_{\mathrm{steric}} 1\, l_{\mathrm{bare}}$. At the upper terrace of the $S^{*}_{\parallel}$ step, the steric repulsion is approximately the same as in the flat surface. Therefore, in this case $l\ (S^{*}_{\parallel})\ '\ l_{\mathrm{bare}}(S^{*}_{\parallel})\ '\ 0.8$ eV. On the other hand, the difference $l\ (S^{*}_{\parallel}) 2\, l(S^{*}_{\perp})\ '\ 1.0\ \mathrm{eV}/a$ reflects approximately $2\, l_{\mathrm{steric}}(S^{*}_{\perp})$ @since the steric repulsion is absent at the $S^{*}_{\perp}$ edge, row a in Fig. 2~a!#. This $2\, l_{\mathrm{steric}}(S^{*}_{\perp})$ $'\ 1.0\ \mathrm{eV}/a$ translates into 1.0 eV/at at the step, which can be compared to the energy gain ~0.18 eV/at! due to the rotation of dihydrides on flat surfaces[10] ~which is a *partial* steric energy gain minus the elastic cost of the rotation!. When the *full* steric energy is removed from the $S^{*}_{\perp}$ step, its formation energy becomes negative. ~ii! Note in Fig. 2~b! that at the center of the terrace, the rotation of the dihydrides is parted into two regions. This division creates extra space that also reduces the steric energy. This effect is not present at the $S^{*}_{\perp} 1 S^{*}_{\parallel}$ structure @see Fig. 2~a!#. Accordingly, the formation energy of the *isolated* $S^{*}_{\perp}$ might be one-tenth of an eV higher than the one estimated here from $S^{*}_{\perp} 1 S^{*}_{\perp}$.

Figure 2~c! shows the $D^{*}_{\perp}$ step with a dihydride configuration similar to $S^{*}_{\perp}$ @see row a in Figs. 2~c! and 2~a!#. In contrast to $S^{*}_{\perp}$, we find that $l\ (D^{*}_{\perp})\ .\ 0$. Since the upper terraces of $D^{*}_{\perp}$ and $S^{*}_{\perp}$ have similar structures, one might wonder why the energy costs of the steps are so different. The reasons are the following. ~i! The estimated $l_{\mathrm{bare}}(D^{*}_{\perp})$ is close to twice $l_{\mathrm{bare}}(S^{*}_{\parallel})$. ~ii! The structure used to calculate $D^{*}_{\perp}$ does not involve the partition of the dimer rotation angles seen in $S^{*}_{\perp} 1 S^{*}_{\perp}$. ~iii! On the $D_{\perp}$

Oshiyama, we find that in the (2 3 1) phase all steps have positive formation energies, which implies that the flat surface is stable against step formation in the (2 3 1) phase. But our results suggest that the same might not be true for the (3 3 1) phase for H chemicals potentials close to the transition to the (1 3 1) phase.

ACKNOWLEDGMENTS

The authors would like to thank Y. J. Chabal for discus-