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Reply to "Comment on 'Step structure of vicinal Ge(001) surfaces' by T. Sato, T. Sueyoshi, T. Amakusa, M. Iwatsuki and H. Tochihara"

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In the preceding comment of Sato et al., these authors claim that only the rebonded SB step edge is found on the stepped Ge(001) surface. In our paper [1] we have concluded that the SB step on the Ge(001) surface exhibits both the rebonded as well as the nonbonded configuration [2]. Sato and co-workers agree with us in so far that they also discern two configurations in their STM images, namely a uniformly rebonded SB step (ur-SB step) and an isolatedly rebonded SB step (ir-SB step). The ur-SB step corresponds with what we have denoted as the rebonded SB step.

For the nonbonded SB step we have proposed two configurations: one configuration has a shifted dimer, the other one is made up of kinks of length $2 \times a_0$ and is oriented along the [010] direction. Sato and co-workers also discern these configurations but they argue that these configurations correspond to the ir-SB step. So, there is consensus about what we have denoted as the rebonded SB step, and the disagreement is about whether the two configurations of the nonbonded SB step are actually nonbonded or of the ir-SB type.

Sato and co-workers use the following argument that the nonbonded SB edges are in fact isolatedly rebonded SB edges: In front of the nonbonded SB step there is an additional dimer which is dark in the filled-state image but bright in the empty-state image. According to Sato et al., we have missed this additional dimer and mistakenly assumed the ir-SB step to be of the nonbonded type, as we have only measured the empty-state images.

Sato and co-workers show STM images with a fine resolution and the discussion is not about the measurements themselves. We disagree, however, with their interpretation of the bright features in the empty-state images as being due to an additional dimer, for the following reasons:

Firstly, at a bias voltage of -2.0 V as we have used, as well as at a bias voltage of -0.8 V as used by Sato et al., the filled states are probed with the STM tip. Formation of a dimer gives rise to a filled state at the dimer bond. Hence, if there is an additional dimer in front of the nonbonded SB step, then it should certainly appear as a protrusion in the filled-state images. These protrusions are absent though in the filled state images of both Sato et al. and ours.

To illustrate this we have plotted an STM image of the Ge(001) surface misoriented towards the [110] direction in Fig. 1. The character 'A' denotes a piece of nonbonded SB step (ir-SB step) which is accompanied on the left hand side by a kink of length

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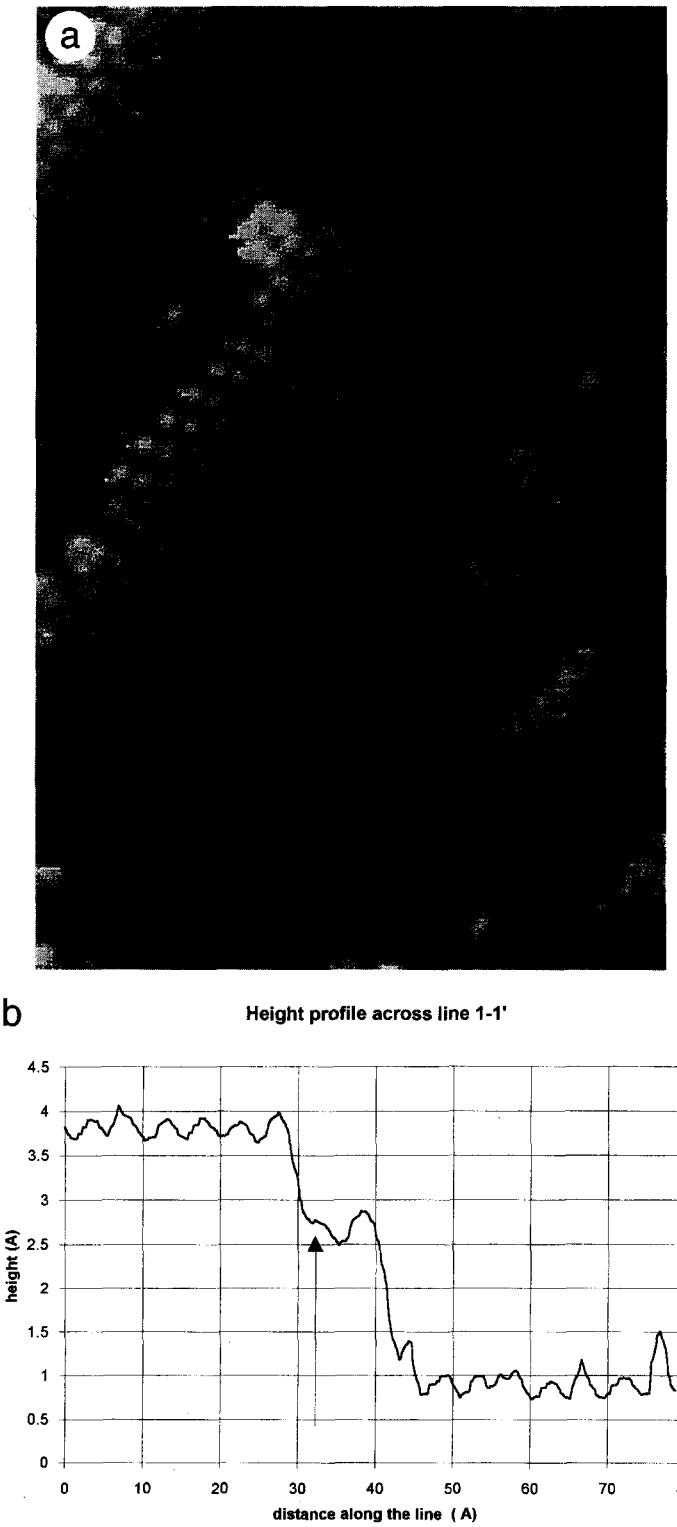

Fig. 1. (a) STM image of Ge(001) misoriented towards the [110] direction by 3°. Scanwidth is 150×226 Å^2, tunnelling voltage is -2 V, i.e. filled states are probed. 'A': piece of nonbonded (ir-) SB step. 'B': piece of nonbonded (ir-) SB step with a shifted dimer. 'C': (uniformly) rebonded SB step. (b), (c), (d): height profiles along lines 1–1′, 2–2′ and 3–3′, respectively. The location of the additional dimer according to Sato et al., is indicated by an arrow in these height profiles.

$2 \times a_0$, the character 'B' denotes a nonbonded SB step (ir-SB step) with a shifted dimer, the character 'C' denotes the (uniformly) rebonded SB step. In Fig. 1b we have drawn the height profile along line 1–1′, parallel to the dimer row of the nonbonded (ir-) SB step. The place where the additional dimer should appear as a protrusion according to Sato et al., is indicated by an arrow. Instead of a protrusion, a

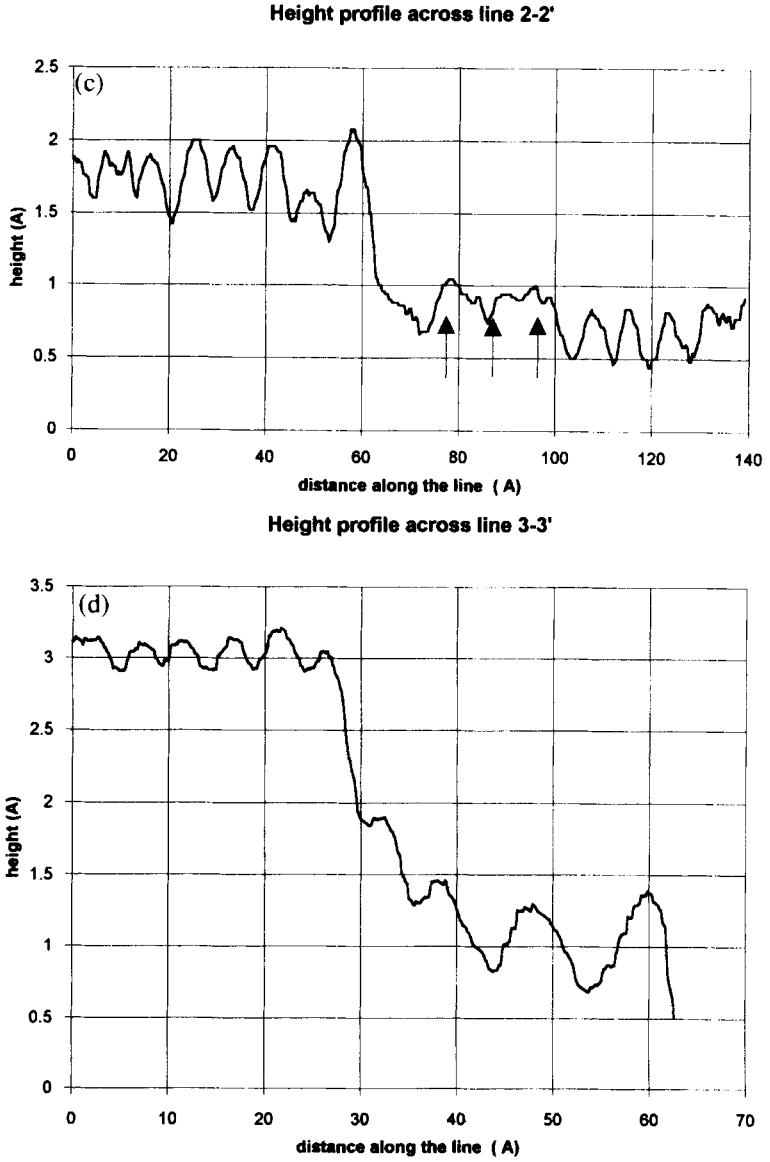

Fig. 1. Continued).

rapid decrease of approximately 1 Å at the location of the additional dimer is observed. Notably, this height profile is not significantly different from the height profile in Fig. 1d, which is along line 3–3′ at 'C' and across the (uniformly) rebonded SB step. The same observation can be made in Fig. 1c, where we have drawn the height profile along line 2–2′ in front of the 'B' step edge. Again, at the place where protrusions are to be expected according to Sato et al., a gap is found of approximately 1 Å with respect to the dimers of the neighbouring terrace.

To illustrate the second argument why we think that such an additional dimer is absent, we have drawn the configuration of the rebonded as well as the nonbonded SB step in Fig. 2. The location of the additional dimer is indicated by an "*", the upward buckled atoms are indicated by a dot. Previously we have argued that the nonbonded SB step gives rise to ferromagnetic buckling of the dimers on the lower terrace in front of the edge dimer. The upward buckled atoms of this ferromagnetic buckling are denoted by 'c'. The ferromagnetic buckling induces anti-ferromagnetic buckling of the dimers lying in front of the neighbouring rebonded SB step. The upward buckled atoms of these dimers are denoted with 'a' in Fig. 2.

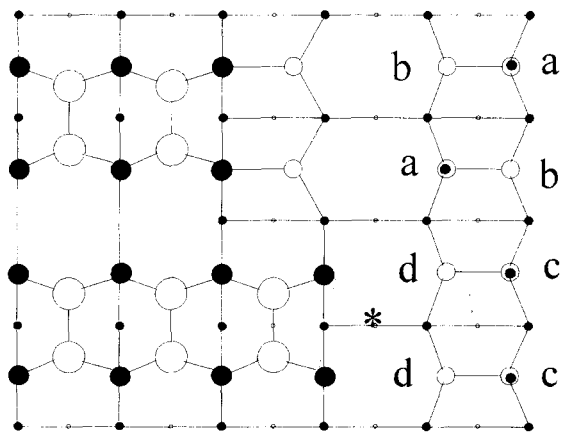

Fig. 2. Configurations of both the rebonded SB edges (above) and the nonbonded SB edges (below) according to Chadi [2]. The atoms buckled out of the surface are indicated by a dot. The '*' denotes the place where the additional dimer, which is claimed by Sato et al., is located.

Kubby et al. investigated the Ge(001) surface with STM by probing both the filled and the empty states [3]. They argued that the buckling of the dimer is accompanied by a filled dangling bond at the atom buckled out of the substrate and an empty, anti-bonding orbital at the atom buckled towards the bulk. By changing the tunnelling voltage they showed that the upward buckled atoms arise as protrusions in the filled-state images and holes in the empty-state images. For the downward buckled atoms the situation is just reversed. The same observation can be made in the filled and empty state images of Sato and co-workers (see Figs. 2a and 2b in their comment). More specifically, turning to our Fig. 2, the atoms 'a' appear as bright in the filled-state images, and dark in the empty-state images of Sato et al., whereas the opposite holds for the atoms denoted 'b' in our Fig. 2. A similar behaviour can be noticed for the atoms denoted with 'c' in Fig. 2 of this reply.

Sato et al. concluded that we misjudged the adatoms of the ir-SB step to be the ferromagnetic buckling. We would like to point out however that these 'c' atoms (Fig. 2) exhibit the same behaviour as the other upward buckled atoms. They, or rather their filled dangling bonds, are visible as protrusions in the filled-state images and holes in the empty-state images of Sato et al. Consequently, it is natural to assume that the 'c' atoms are accompanied by downward buckled atoms, denoted 'd' in Fig. 2 of our reply. As the anti-bonding orbitals are located at the downward buckled atoms, these 'd' atoms should appear as protrusions in the empty-state image. Our interpretation of the bright feature which Sato et al. observe in the empty-state images at 'd' (Fig. 2), is that it is not a dimer but represents the anti-bonding orbitals of the ferromagnetic buckling. Notably we would like to remark that the additional dimers in the empty-state images in Fig. 2 of the comment of Sato et al., seem somewhat smaller and lower than the dimers of the higher terrace.

In conclusion: Sato and co-workers observe protrusions in front of the nonbonded SB step in the empty-state STM images. From this they conclude that there is an additional dimer at the nonbonded SB step and that consequently the nonbonded SB step is actually a rebonded one. We disagree about the

existence of an additional dimer, as instead of protrusions, holes are found in the filled-state images. Here, we propose that the protrusions in the empty-state images are the anti-bonding orbitals of the ferromagnetic buckled dimers in accordance with observations of Kubby et al. [3].

References

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