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Erratum: Step energy and step interactions on the reconstructed GaAs(001) surface (Physical Review B - Condensed Matter and Materials Physics (2014) 90 (115314) DOI: 10.1103/PhysRevB.90.115314)

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# ERRATUM: Step Energy and step interaction on the reconstructed GaAs(001) surface [Phys. Rev. B 90,115314 (2014)]

Rita Magri, Sanjeev K. Gupta, and Marcello Rosini

(Dated: December 5, 2016)

## Abstract

We correct here the values obtained in our paper [R. Magri, S. K. Gupta, and M. Rosini, Physical Review B 90, 115314 (2014)] regarding the surface energies of vicinal surfaces to the GaAs(001)  $\beta_2(2 \times 4)$  reconstructed surface. The calculations were performed using an ab-initio density functional method and were affected by a wrong choice for the value of the input parameter governing the occupation broadening of the electronic states around the Fermi energy. We have carefully checked the effect of this parameter on the calculated values and found a converged value, thus mending our previous values for the step energies and the step interactions of the many step configurations considered in the paper. As a consequence we find now that the step configuration less unstable and thus more likely to be experimentally observed is just the one which was actually seen by STM<sup>1</sup> putting our calculations in agreement with the experiment.

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We report here the corrected values for the step energies and the step interactions calculated in our previous paper<sup>2</sup> for a large set of different step configurations. We have found that one parameter, i. e. the smearing parameter governing the band occupation around the Fermi level, was not converged enough to predict the step properties with sufficient accuracy. Since the surfaces are metallic a smearing function had to be used for the state occupation around the Fermi level. We used the smearing function proposed by Marzari and Vanderbilt<sup>3</sup>. We found that the parameter  $\Delta$  (*degauss*) entering this expression is a particularly sensitive one. The previous paper used a commonly chosen value of 0.02 Ry. However, we found that a much smaller value for this parameter was necessary to obtain well converged values for the surface energies.

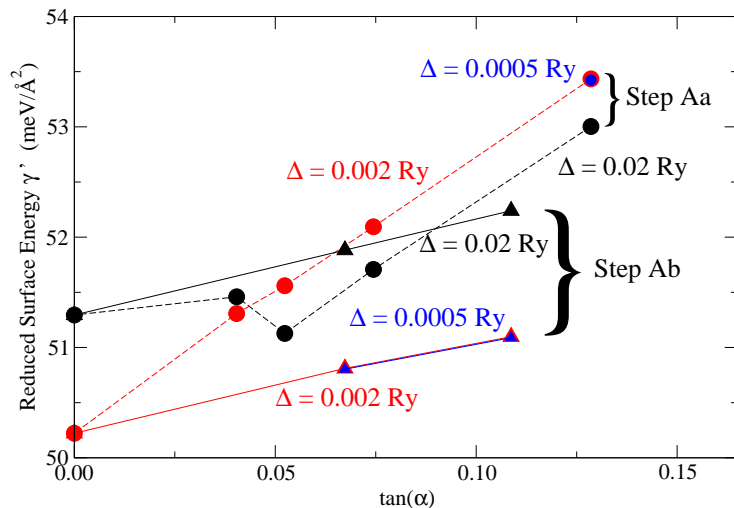


Figure 1. (Color online) Reduced surface energy  $\gamma'$  versus miscut angle  $\tan(\alpha)$  obtained using different values for the input parameter  $\Delta$ . Black symbols:  $\Delta = 0.02$  Ry. Red symbols:  $\Delta = 0.002$  Ry. Blue symbols:  $\Delta = 0.0005$  Ry. Dots: steps *Aa*, triangles: steps *Ab*. The dashed lines (step *Aa*) and the solid lines (step *Ab*) are for guiding the eye.

The convergence of the smearing parameter has been carefully checked. We report in Fig. 1 the calculated values of the reduced surface energies of the vicinal surfaces with steps of kind *Aa* and *Ab* using the old (0.02 Ry) and the new (0.002 Ry) value for the  $\Delta$  parameter as a function of the miscut angle. The figure shows also that the new value produces surface energies well converged with respect to the  $\Delta$  parameter. Reducing further this parameter to 0.0005 Ry produces indeed no significant changes in the calculated surface energies.

The choice of a smaller value for this parameter arises problems relative to the correct

integration of the electronic charge around the Fermi energy. Thus, also the choice of the k-point grid for the Brillouin Zone integrations needs to be revisited accordingly. We tested the convergence of the results versus the number of k points and found that the k-point grid used in Ref. 2 was sufficient to obtain converged results also when a smaller smearing parameter is used. Thus, we found that the only notable source of error in our previously calculated values was only the too large value of the smearing parameter  $\Delta$ .

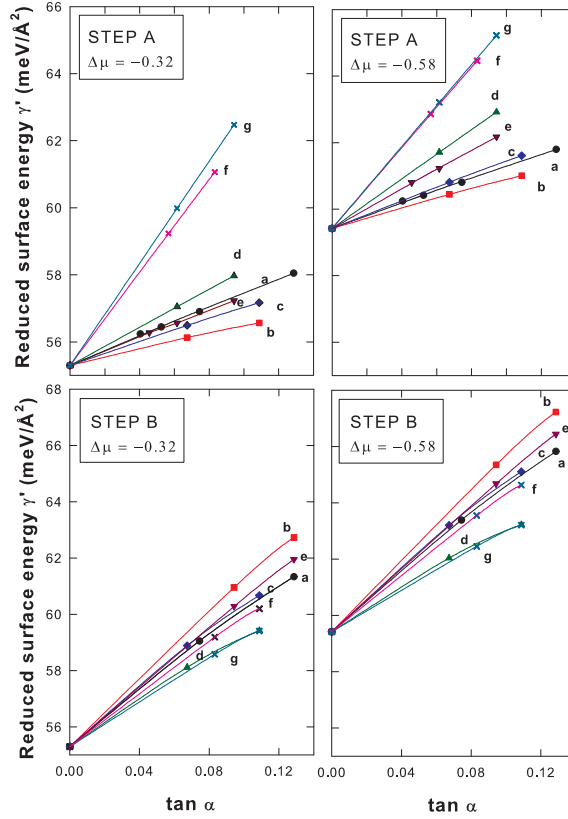


Figure 2. (Color online) Reduced surface energies versus miscut angles  $\tan\alpha$  for steps A and B at  $\Delta\mu_{As} = -0.32$  and  $\Delta\mu_{As} = -0.58$ . This figure corresponds to Fig. 3 of Ref 2.

We report next the corrected version of Fig. 3 of Ref 2. The Figure shows the recalculated reduced surface energies of many step configurations of both kind A (oriented like the As surface dimers) and kind B (oriented perpendicular to the As surface dimers).

The most noticeable change is that the step *Ab* is now the configuration having the lowest step energy, thus it is the configuration that should be seen experimentally, as it is the case<sup>1</sup>. Also, the ratio between the step energy of the lowest energy step of kind B (the step *Bg*)

and the  $Ab$  step at  $\Delta\mu_{As} = 0$  is about 5 in reasonable agreement with the experimental reported value of about 6<sup>4</sup>.

STEPS A							
	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$\epsilon(\Delta\mu_{As} = 0)$ (meV/Å)	72.4	25.6	40.6	49.9	29.3	225.7	264.5
$\epsilon(\Delta\mu_{As} = -0.32)$ (meV/Å)	62.4	35.7	50.7	80.1	59.6	195.6	214.1
$\epsilon(\Delta\mu_{As} = -0.58)$ (meV/Å)	54.1	44.0	58.9	104.7	84.1	171.0	173.2
$q$ (meV/Å)	-52	-92	-73	-22	-90	-53	-21
$K_{el}$ (meV/Å)	+50.78	-	-	-	+168.81	-	-
STEPS B							
	$a$	$b$	$c$	$d$	$e$	$f$	$g$
$\epsilon(\Delta\mu_{As} = 0)$ (meV/Å)	136.3	165.5	146.4	134.4	141.9	128.0	127.1

Table I. Step parameters for the A and B steps of kind  $a, b, c, d, e, f, g$ .  $\epsilon$  is the step energy for different values of the Arsenic chemical potential  $\Delta\mu_{As}$  while  $q$  are the values of the step-step interaction.  $K_{el}$  is the estimated elastic constant  $K$  of the  $K/L^2$  step-step interaction term. The other parameters listed in Table I of Ref. 2 are unaffected by the different values of the ab-initio calculated surface energies.

We report also in Table I the corrected values of the step energies  $\epsilon$ , the step interaction parameters  $q$ , and the coefficients  $K_{el}$  of Table I of Ref. 2. All the other data reported in the Table are parameters independent from the ab-initio calculated surface energies.

Next, we report in Fig. 3 the corrected version of Fig. 4 of Ref. 2.

This figure shows that in the case of the step  $Ae$  all four values, including  $\gamma_{\beta_2}$ , are necessary to provide a good estimation for the step energy  $\epsilon$ .

Finally, we show in Figs. 4 and 5 the averaged (over the first six atomic planes) displacements  $U_x$  and  $U_z$  obtained using the converged  $\Delta$  parameter (black lines and symbols) compared with the previous values reported in Fig. 6 and Fig. 7 of Ref. 2 (green lines and symbols). The re-calculated averaged atomic displacements have been fit using Eq. (4) or Ref. 2. The fitted elastic dipole forces of the standard model<sup>5</sup> are reported in the captions of the figures.

While the general picture has not changed we can notice that in the case of step  $Aa$  the

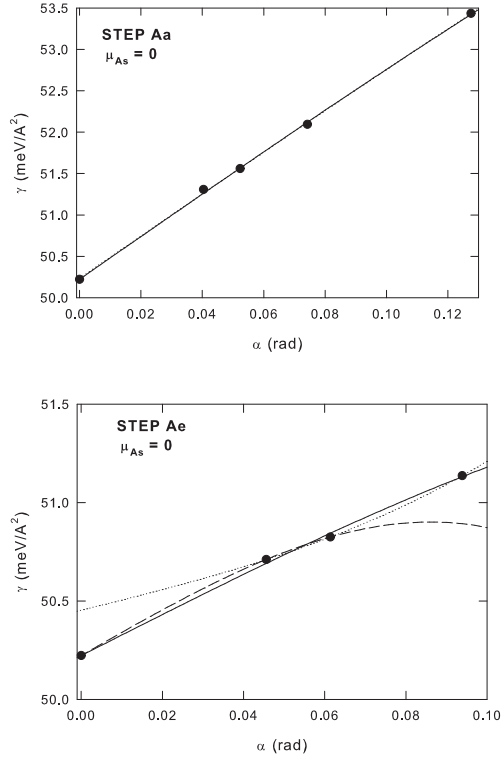


Figure 3. (Color online) Above: step *Aa*. Solid line: all five values,  $\epsilon = 72.4 \text{ meV}/\text{\AA}$ ,  $q = -52 \text{ meV}/\text{\AA}^2$ ; dotted line: four values without  $\gamma_{\beta_2}$ ,  $\epsilon = 71.6 \text{ meV}/\text{\AA}$ ,  $q = -36 \text{ meV}/\text{\AA}^2$ , predicted  $\gamma_{\beta_2} = 50.24$  (calculated value  $50.22$ )  $\text{meV}/\text{\AA}^2$ , dashed line: four values including  $\gamma_{\beta_2}$  and excluding the shorter step distance, no difference with the fit using all five values. Below: step *Ae*. Solid line: all four values,  $\epsilon = 29.3 \text{ meV}/\text{\AA}$ ,  $q = -90 \text{ meV}/\text{\AA}^2$ ; dotted line: three values without  $\gamma_{\beta_2}$ ,  $\epsilon = 14.5 \text{ meV}/\text{\AA}$ ,  $q = +238 \text{ meV}/\text{\AA}^2$ , predicted  $\gamma_{\beta_2} = 50.45 \text{ meV}/\text{\AA}^2$ , dashed line: three values including  $\gamma_{\beta_2}$  and excluding the shorter step distance,  $\epsilon = 33.1 \text{ meV}/\text{\AA}$ ,  $q = -529 \text{ meV}/\text{\AA}^2$ .

displacements are larger closer to the step and smaller on the terraces compared with those obtained in the previous calculation of Ref. 2. In the case of the step *Ae* instead the newly calculated displacements are smaller everywhere.

In the light of these new results some of the conclusions of the paper need to be re-addressed. First, the less unstable A step configuration is not the Ga-rich *Aa* step but is the As-rich *Ab* step which was actually the observed step configuration in the experiment by Kanisawa et al.<sup>1</sup>. Those authors indeed observed step edges having the atomic structure

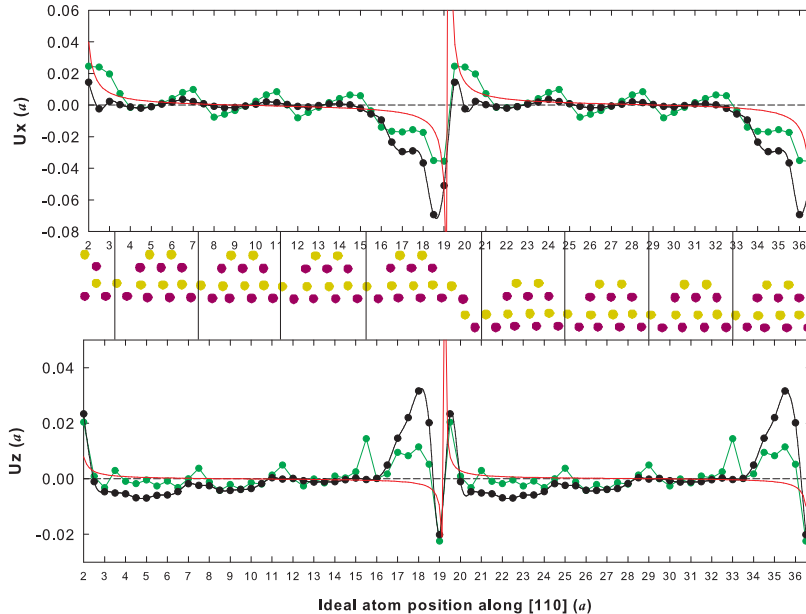


Figure 4. (Color online) (a)  $U_x$  and (b)  $U_z$  of step  $Aa$  at the atomic positions  $na$  along the  $[110]$  direction.  $a = 3.97\text{\AA}$  is the surface lattice parameter. The black symbols and lines are the recalculated values, the green symbols and lines are the values of Ref. 2. Red line: fit of  $U_x$  and  $U_z$  using the Eq. (4) of Ref. 2. The obtained values for the force dipole components are  $A_x = -166\text{ meV/\AA}$  and  $A_z = -32.77\text{ meV/\AA}$ . In the middle is a ball and stick side view of the surface atomic layers; yellow dots: As atoms; purple dots: Ga atoms.

corresponding to the As-rich  $Ab$  step on  $\beta_2(2\times 4)/c(2\times 8)$  reconstructed vicinal surfaces using ultra-high vacuum scanning tunneling microscopy (STM). Second, the step-step interactions extracted by fitting the corrected surface energies are all attractive. They tend to be more attractive for the As-rich steps (apart the noticeable exception of the  $Ae$  steps) than for the Ga-rich steps. While the possible connection of the step interaction with the step electronic structure is not anymore evident from the corrected values the discrepancy with the classical elastic model of step interaction predicting always repulsive interactions for like-oriented steps still holds.

## ACKNOWLEDGMENTS

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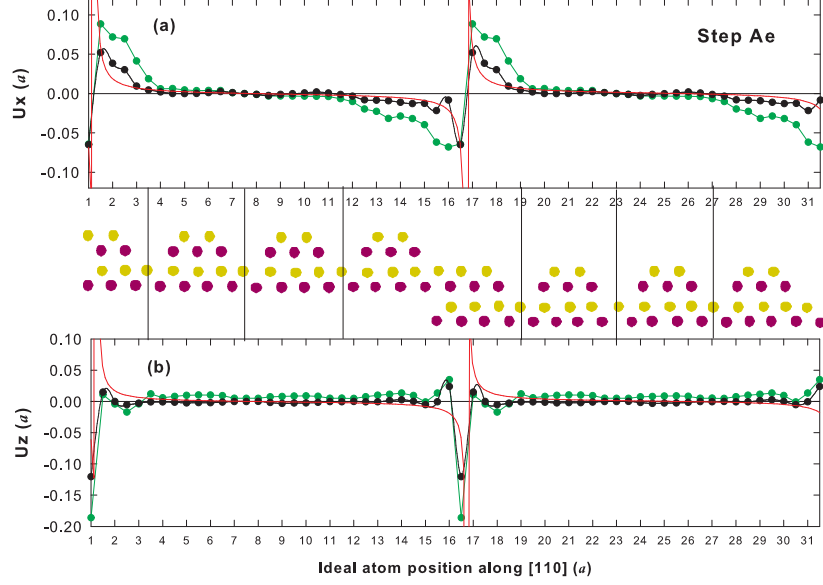


Figure 5. (Color online) (a)  $U_x$  and (b)  $U_z$  of step  $Ae$  at the atomic positions  $na$  along the  $[110]$  direction.  $a = 3.97\text{\AA}$  is the surface lattice parameter. The black symbols and lines are the recalculated values, the green symbols and lines are the values of Ref. 2. Red line: fit of  $U_x$  and  $U_z$  using Eq. (4) of Ref. 2. The obtained values for the force dipole components are  $A_x = -229.52 \text{ meV/\AA}$  and  $A_z = -206.12 \text{ meV/\AA}$ . In the middle is a ball and stick side view of the surface atomic layers; yellow dots: As atoms; purple dots: Ga atoms.

The authors are indebted to Prof. Anna Franchini and Ms. Giulia Righi for the calculation of the corrected surface energies.

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<sup>1</sup> K. Kanisawa, H. Yamaguchi, and Y. Horikoshi, Phys. Rev. B **54**, 4428 (1996).

<sup>2</sup> R. Magri, S. K. Gupta, and M. Rosini, Phys. Rev. B **90**, 115314 (2014).

<sup>3</sup> N. Marzari, D. Vanderbilt, A. De Vita, and M. C. Payne, Phys. Rev. Lett. **82**, 3296 (1999).

<sup>4</sup> E. J. Heller, Z. Y. Zhang, and M. G. Lagally, Phys. Rev. Lett. **71**, 743 (1993).

<sup>5</sup> V. I. Marchenko, and A. Y. Parshin, Sov. Phys. JETP **52**, 129 (1980).