Erratum:

Thermodynamics and Statistical Mechanics of the Faceting of Stepped Si(111)

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A correction is needed in equations 25a and 25b, which give the contribution of step-step interaction to the surface free energy in terms of the step diffusivity [1]. Due to an inconsistent factor of two in a source reference [2], our equations include a factor of two error in the contribution of the step diffusivity, b^2. Thus, the correct form of the equation 25a is:

$$g(\theta,T)=\frac{\pi^2 kTb^2(\theta,T)}{24a_p h^3}\left\{1+\left[1+\frac{4Aa_p}{kTb^2(\theta,T)}\right]^{1/2}\right\}^2 \qquad (25a)$$

for step-step interactions of the form $U(x)=A/x^2$. The correct form for Eq. 25a, for the case of no energetic step-step interactions, $A = 0$, is now consistent with reference [3],

$$g(\theta,T)=\frac{\pi^2 kTb^2(\theta,T)}{6a_p h^3}. \qquad (25b)$$

The incorrect forms of these equations have also been used in previous publications [4,5].

In addition, the previously reported value of the step stiffness, $\tilde{\beta}$, for the high-temperature phase [6], which was used in our numerical analysis in [1], has been found to be half of the correct value [7]. We have repeated our numerical analysis using both the corrected version of Eq. 25a, and the corrected value of the step stiffness. When we use the corrected value of the stiffness, $\tilde{\beta} \approx 0.14$ eV/Å, we obtain a value for the step diffusivity of $b^2(900^{\circ}\mathrm{C}) \approx 2.85\,\text{Å}^2$, which is half the value used previously [1]. The resulting values of the step interaction coefficient, g, calculated from the corrected Eq. 25a at 900°C are thus unchanged. However, the kink energy consistent with the corrected value of the step stiffness is now $\varepsilon \approx 0.23$ eV for the high-temperature phase, and thus the temperature dependence of Eq. 25 is different. Repeating the numerical analysis of the experimental data gives the following results:

Phase separation along [$\bar{2}11$] and [$1\bar{1}0$]

The values previously reported in Table 2 [1] are unchanged except for the absolute value of the step energy in the high-temperature phase, which increases to 55-58 meV/Å. The difference in step energies between the 7x7 and 1x1 phase is the same as previously reported, so that the absolute value of the step energy in the 7x7 phase becomes $\beta_b(0,T) \gtrsim 70$ meV/Å, or 1.9 eV per 7x7 unit-cell edge. In the isotropic sqaure-lattice model for step/kink energies, this number would also give the kink energy in the 7x7 phase of approximately 1.9 eV.

Phase separation along [$2\bar{1}\bar{1}$] $\pm\theta$

The values in tables 3 and 4 [1] which involve rotations of the step edge are larger in magnitude, due to the larger kink energy. However, the calculated difference in step energies between the two phases remains small. The absolute values of the step energies along the [$2\bar{1}\bar{1}$] azimuth phases is larger for both phases; for the 7x7 phase, $\beta_{\mathrm{b}}^{\mathrm{triple}} \approx 165$ meV/Å, and $\beta_{\mathrm{b}}^{\mathrm{single}} \approx$ 55 meV/Å, and for the high-temperature phase, $\beta_{\mathrm{a}}^{\mathrm{single}} \approx 56$–$60$ meV/Å over the temperature range 770-845$^{\mathrm{o}}$C. In the symmetric model for the step, the estimates of the kink energies for both single and triple height steps in the 7x7 phase become $\varepsilon_{\mathrm{b}}^{\mathrm{single}} \approx 1.5$ eV, and $\varepsilon_{\mathrm{b}}^{\mathrm{triple}} \approx 4.4$ eV.

Conclusions

The corrected values for the parameters needed to fit the experimental phase diagrams are listed in the table, which corresponds to the previous Table 5 [1]. As noted previously [1], the absolute values of the step energies are not especially significant, due to the physical limitations of the square-lattice model used in the analysis. The significant results, 1) that the differences in the step energies governing surface stability are governed by the magnitude of the step-step interactions, and 2) that the phase diagram of the vicinal of Si(111) can be described within an internally consistent thermodynamic framework, remain unchanged. The values for the differences in step energies between the 7x7 and high temperature phase, $\Delta\beta > 10$ meV/Å in the [$\bar{2}11$] direction and $\Delta\beta \approx -5$ meV/Å in the [$2\bar{1}\bar{1}$] direction, are the same as previously reported [1].

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References

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Table V Corrected values of the parameters needed to describe the complete phase diagram of Si(111) in a nearest-neighbor square lattice model with elastic step-step interactions.

	7x7 phase		1x1 phase
	$[\bar{2}11]$ azimuth (single height steps)	$[2\bar{1}\bar{1}]$ azimuth (triple height steps)	$[\bar{2}11]$ and $[2\bar{1}\bar{1}]$ azimuth
kink energy, ε	>1.9 eV	4.4 eV	0.23 eV
step-interaction strength, A	0.40 eV-Å	3.6 eV-Å	0.15 eV-Å
step formation energy, $\beta(0,800^{o}C)$ (Eq. 9, 19)	>70 meV/Å	165 meV/Å	56 meV/Å
step-interaction term $g(0,800^{o}C)$ (Eq. 9, 25)	0.022 eV/Å^2	0.007 eV/Å^2	0.014 eV/Å^2