

## COMMENTS

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### Comment on “Step dynamics and equilibrium structure of monoatomic steps on Si(100)-2×1”

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In contrast to a recent claim by Sánchez and Aldao [Phys. Rev. B **54**, R11 058 (1996)] that the relaxation dynamics of attachment processes influences the equilibrium step structure we argue that the step structure in thermodynamic equilibrium is only governed by the configurational free energy regardless of the exact details of the relaxation dynamics. [S0163-1829(97)05331-9]

In a recent paper,<sup>1</sup> Sánchez and Aldao claim that direct application of the Burton, Cabrera, and Frank theory<sup>2</sup> to quenched step patterns of Si(100) leads to incorrect interaction energies. Inspired by high-temperature scanning tunneling microscopy experiments on Si(100) performed by Pearson *et al.*,<sup>3</sup> Sánchez and Aldao claim that the exact nature of relaxation processes of step edge attachment events influence the *equilibrium step edge roughness* of Si(100). By introducing a factor  $R$ , which refers to the relative difference in the strength of two different attachment relaxation processes, in their Monte Carlo simulations, Sánchez and Aldao arrive at the conclusion that the steady-state roughness of the steps depends on  $R$ . Sánchez and Aldao consider only the relaxation dynamics of the attachment events and not of the detachment events. If the relaxation dynamics of detachment events is not taken into account properly, this will result in violation of energy conservation. In order to illustrate our point we reconsider the example (Fig. 3 in Ref. 1) discussed in the paper by Sánchez and Aldao. We use the same nomenclature as Sánchez and Aldao. The barrier for attachment in Fig. 1 is denoted by  $E_1$  and  $E_2$ , respectively (entropy effects are, for simplicity, ignored). The probabilities  $P_{a \rightarrow b}$  and  $P_{b \rightarrow a}$  can be written as

$$P_{a \rightarrow b} = e^{-(E_x + E_y + E_1 + E_2)/kT} \quad \text{and} \quad P_{b \rightarrow a} = e^{-(E_y + E_1 + E_2)/kT}.$$

In agreement with Refs. 2, 4, and 5 the ratio  $P_{a \rightarrow b}/P_{b \rightarrow a}$  is given by  $\exp(-E_x/kT)$ . Therefore, we must conclude that,

provided that the step edges are in *thermodynamic equilibrium*, the kink population statistics will only be governed by the *configurational free energies* regardless of the exact details of the relaxation dynamics.

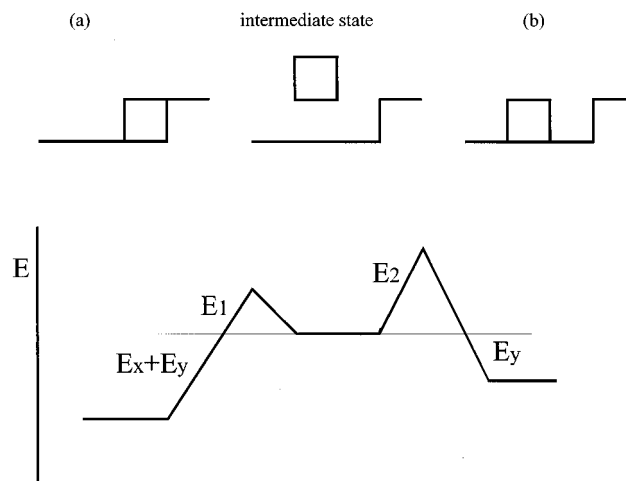


FIG. 1. A schematic diagram depicting a step edge rearrangement process at a step edge. The activation energy for going from state (a) to the intermediate state is  $E_x + E_y + E_1$ . The activation energy for going from state (b) to the intermediate state is  $E_y + E_2$ . The activation energy for going from the intermediate state to state (a) [state (b)] is  $E_1$  ( $E_2$ ).

<sup>1</sup>J. R. Sánchez and C. M. Aldao, Phys. Rev. B **54**, R11 058 (1996).

<sup>2</sup>W. K. Burton, N. Cabrera, and F. C. Frank, Philos. Trans. R. Soc. London, Ser. A **243**, 299 (1951).

<sup>3</sup>C. Pearson, B. Borovsky, M. Krueger, R. Curtis, and E. Ganz, Phys. Rev. Lett. **74**, 2710 (1995).

<sup>4</sup>B. S. Swartzentruber, Y.-W. Mo, R. Kariotis, M. G. Lagally, and M. B. Webb, Phys. Rev. Lett. **65**, 1913 (1990).

<sup>5</sup>H. J. W. Zandvliet, H. B. Elswijk, E. J. van Loenen, and D. Dijkkamp, Phys. Rev. B **45**, 5965 (1992).