Alerhand *et al.* Reply: The principal statement in the preceding Comment[1] regarding a coexistence region in the phase diagram[2] for vicinal Si(100) surfaces would be valid if it were appropriate to treat the surface misorientation angle θ as an *annealed density*. However, in the problem of interest here the angle θ is determined by the original miscut, and it remains constant across the surface. For the time scales in the experiments the mass transport required to change θ does not occur, and faceting is not observed. Thus θ is a *quenched density* for these experiments, which is theoretically equivalent to a thermodynamic field.[3] The phase diagram in the variables of the quenched density and temperature does not have a coexistence (phase-separation) region, but a coexistence line.

The existence of a transition line and the absence of a transition region in the phase diagram of vicinal Si(100), as predicted in our Letter, has been further corroborated in recent experiments by Grundmann, Krost, and Bimberg.[4] They relate the surface morphology at a given temperature and misorientation angle to the presence or absence of antiphase domains in a thin layer of a zinc-blende material (InP) grown on a Si(100) surface. The results are in excellent agreement with our theory. Also, Swartzentruber *et al.*[5] have used a model similar to ours to analyze fluctuations in step profiles observed with a scanning tunneling microscope (STM). They determine experimentally the energetics associated with kinks, and from this they infer step and corner energies (the latter not treated in our Letter).

Further evidence that the proposed model properly describes the behavior of steps on Si(100) is given in Figs. 1 and 2. Figure 1 shows profiles of meandering *SB*-type steps obtained from Monte Carlo simulations of the step

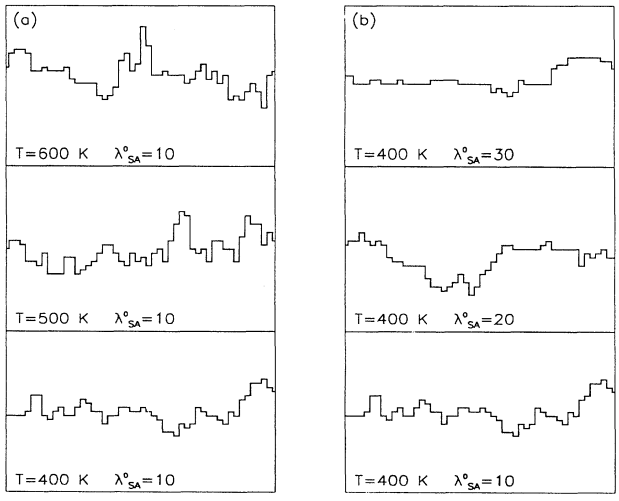

FIG. 1. Monte Carlo simulations of meandering *SB*-type steps (1° surface misorientation, distance between horizontal lines drawn to scale). (a) Step profiles at $T=400$, 500, and 600 K, with $\lambda^0_{SA}=10$ meV/a. (b) Step profiles for $\lambda^0_{SA}=10$, 20, and 30 meV/a at $T=400$ K.

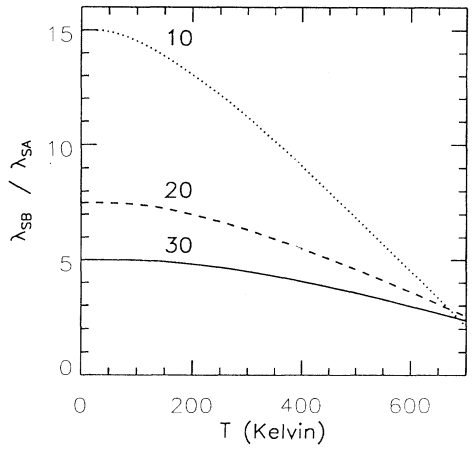

FIG. 2. Ratio of step free energies $\lambda_{SB}/\lambda_{SA}$ vs temperature. Dotted, dashed, and solid lines correspond to $\lambda^0_{SA}=10$, 20, and 30 meV/a, respectively.

Hamiltonian given by Eq. (4) in our Letter. These are in good agreement with STM images[2,5] of the surface. New experimental evidence[4,5] suggests that the energy of *SA*-type steps is larger than the calculated value of $\lambda^0_{SA}=10$ meV/a previously used ($a=3.84$ Å is the step unit length). This is the dominant energy in the fluctuations. Accordingly, Figs. 1 and 2 show results for a range of energies that should include the correct value (in very good comparison, for example, with Fig. 1 of Ref. 5). Figure 2 shows the calculated ratio of free energies $\lambda_{SB}/\lambda_{SA}$ for the two types of single-layer steps on Si(100). This determines the shape of equilibrium two-dimensional islands of Si deposited on Si(100).[5]

O. L. Alerhand
Bellcore
Red Bank, New Jersey 07701

A. Nihat Berker and J. D. Joannopoulos
Department of Physics, Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

David Vanderbilt
Department of Physics, Harvard University
Cambridge, Massachusetts 02138

R. J. Hamers and J. E. Demuth
IBM Research Division, T. J. Watson Research Center
Yorktown Heights, New York 10598

Received 20 September 1990
PACS numbers: 68.35.Bs, 61.16.Di, 64.80.Gd, 81.40.Ef

[1]N. C. Bartelt, T. L. Einstein, and C. Rottman, preceding Comment, Phys. Rev. Lett. **66**, 961 (1991).

[2]O. L. Alerhand *et al.*, Phys. Rev. Lett. **64**, 2406 (1990).

[3]See, for example, D. Andelman and A. N. Berker, Phys. Rev. B **29**, 2630 (1984).

[4]M. Grundmann, A. Krost, and D. Bimberg, Technical University of Berlin report, 1990 (to be published).

[5]B. S. Swartzentruber *et al.*, Phys. Rev. Lett. **65**, 1913 (1990); M. G. Lagally *et al.*, in *Kinetics of Ordering and Growth at Surfaces,* edited by M. G. Lagally (Plenum, New York, 1990).