Robinson, Vlieg, and Kern Reply: A new model of the Pt(110) surface phase transition is proposed in the preceding Comment by Vilfan and Villain.[1] The model is a 2D Ising model on a flat substrate in which the domain walls are pairs of steps bound together.

We showed in our original paper[2] that the presence of steps between neighboring reconstructed regions of the surface gives an approximately Lorentzian diffraction profile which is shifted from the exact half-order position expected for the reconstruction. The new derivation[1] shows this result is also correct in the case of step pairs. We parametrized the experimentally observable features of peak position and peak width in terms of two surface densities: that of isolated steps (denoted α) and that of antiphase domain walls with zero width (β). Vilfan and Villain[1] consider the steps to be always paired into antiphase domain walls, now extended in size (see Fig. 1 in the preceding Comment), and so introduce instead the density ($1/\xi$) and the width (l) of walls as parameters. Although the two descriptions differ in the assumed correlations between the steps, this should not lead to a big difference in the diffraction line shape: Either parametrization is consistent with the basic features of the experimental line shape.

The implications for the mechanism of the phase transition are very different for the two models, however. This is manifested in the temperature dependence of the derived parameters, which we measured.[2] If, as we originally suggested, the unbound steps are present with a random sense (up or down) on the surface, it is rough by definition. The phase transition at 1080 K leading to this state would then be a roughening transition, and would be expected to have different critical behavior (if any) from what we observed.[2] On the other hand, the imposition of step pairing leads to a model in the Ising universality class. This proposition is attractive because our observed experimental values of the critical exponents, $\beta_0 = 0.11 \pm 0.01$ and $\nu = 0.95 \pm 0.09$, are consistent with the theoretical values $\beta_0 = \frac{1}{8}$ and $\nu = 1$ for the 2D Ising model. We therefore prefer the new suggestion of step pairs because of its better account of the observed critical behavior.

At the quantitative level, the new model has some possible problems. First of all, the calculated line shape in Eq. (4) of Ref. 1 fits the observed peaks rather poorly: The curves, especially for the higher-temperature values, are extremely distorted and can become negative on the side opposite the shift. This must be due to a poor approximation, since the pairing of steps should only subtly change the description we presented.[2]

Second, if the wall thickness l were determined by the local interactions between the pair of steps, it would not be expected to have a strong temperature dependence, whereas the correlation length ξ diverges critically at T_c. Experimentally, both the peak shift and linewidth vary linearly[2] with $t = T/T_c - 1$, which, according to the new model,[1] implies $l(t) \propto \xi(t) \propto 1/t$. The implication that the walls contract with increasing T is a little counterintuitive: We might expect instead that roughening would eventually take place, at higher temperatures still, by an *unbinding* of the step pairs. Moreover in the new model, when T_c is approached from above, $l(t)$ diverges, the steps effectively unbind, and more steps could nucleate within the retreating walls to roughen the surface as T is *reduced* towards T_c.

What is called for now is another experiment to test these predictions. It should be possible to measure the temperature dependence of the integer-order diffraction-peak profiles (crystal truncation rods) which are very sensitive to surface roughness.[3] If the new model[1] is right, no change should be seen; the old model,[2] which assumes no interactions between the steps, predicts an observable increase of roughness above T_c.

I. K. Robinson,[(1)] E. Vlieg,[(1)] and K. Kern[(1),(2)]
[(1)]AT&T Bell Laboratories
Murray Hill, New Jersey 07974
[(2)]Institut für Grenzflächenforschung und Vakuumphysik
Kernforschungsanlage Jülich
Postfach 1913, 5170 Julich, West Germany

Received 18 June 1990
PACS numbers: 68.35.Bs, 05.50.+q, 61.50.Ks

[1]I. Vilfan and J. Villain, preceding Comment, Phys. Rev. Lett. **65**, 1830 (1990).
[2]I. K. Robinson, E. Vlieg, and K. Kern, Phys. Rev. Lett. **63**, 2578 (1989).
[3]I. K. Robinson, Phys. Rev. B **33**, 3830 (1986).