

Surface Stress and Self-Organization of Steps

In a recent Letter, Hanesch and Bertel [1] (HB) report a spontaneous modulation of the Pt(110) surface. Their discovery is fascinating. However, the interpretation requires revision. A uniform surface stress could not, by itself, account for this self-organization of steps. Moreover, the inferences regarding the magnitude of the surface stress, based on the structure, are unjustified. These issues of interpretation and analysis do not detract from the importance of the discovery.

HB reported spontaneous formation and self-organization of steps on Pt(110), and attributed this to the large surface stress. Adapting an analysis by Tersoff and Tromp [2] for strained layers (i.e., *bulk* stress), they argued that the absolute surface stress can be inferred from the self-organized structure. But the effects of surface and bulk stress are actually quite different.

A bulk stress gives rise to a “force monopole” at a step, as shown schematically in Fig. 1(a) for the case of compressive stress. At the step, there is compressed material on the left and not on the right, so there is a net elastic force to the right. This net force can lead to negative step formation energies [3], logarithmic attraction and step bunching [4], and even self-organization during step-flow growth [5].

In contrast, a uniform surface stress gives rise only to a “force dipole” at the step [6], illustrated in Fig. 1(b) for the case of a compressive surface stress. The upper and lower terraces apply equal and opposite forces to the step, displaced relative to each other by the step height. This corresponds to a force dipole with the character of a torque

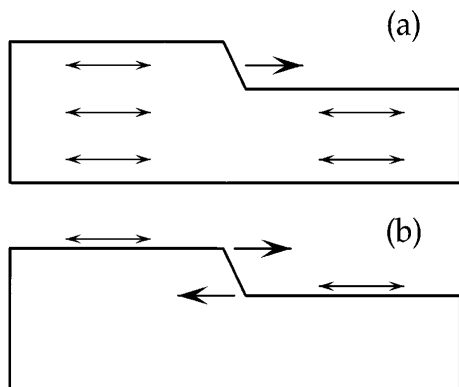


FIG. 1. Schematic illustration of stresses and forces, for the case of (a) bulk stress, and (b) surface stress. (a) Double arrows represent bulk compressive stress. There is more material, and therefore more stress, on the left than on the right. This leads to a net force (a “force monopole”) at the step, indicated by the single arrow. (b) Double arrows represent surface compressive stress. The presence of a surface at a given level on the left, but not on the right, causes a force shown by the upper arrow. The termination of the surface on the opposite side of the step creates an equal and opposite force, displaced vertically. This pair of opposite forces represents a “force dipole.”

or shear stress. A step may also have an additional force dipole, with the character of a diagonal stress, due to its microscopic properties [6].

In the absence of bulk stress or other complications, the energy of an ensemble of steps is then [6]

$$E = \sum_m C_0 + \sum_{m \neq n} (C_{xx} + s_m s_n C_{xy}) (x_m - x_n)^{-2}. \quad (1)$$

Here, x_m is the position of the m th step, and s_m is its sign (± 1 for up or down); C_{xy} is the torquelike force dipole term, proportional to the square of the surface stress; and the dipole C_{xx} is a local property of the step itself.

The step formation energy C_0 could, in principle, be negative, and HB recognize that this is more likely in the case of a large surface stress. But this alone could not account for the experimental observations. For $C_0 < 0$ and $C_{xx} > C_{xy}$, the minimum-energy structure corresponds to alternating up and down steps, equally spaced. This would indeed be self-organization; but it is not the structure observed. [For $C_{xy} > C_{xx}$, the surface is unstable according to [1]; but this reflects the breakdown of that asymptotic linear form when the steps are atomically close. In this case, one might expect some surface reconstruction, such as occurs for Au(110), which could be viewed as stress-induced self-organization. Or the reduction of the interaction by elastic nonlinearity, etc., might eliminate the instability.]

If, rather than having independent steps, the surface is faceted, a uniform surface stress could lead to self-organization [7]. Then it is the stress *in the facet plane*, not the stress of the (110) terrace, which is relevant.

The actual cause of the observed self-organization for Pt(110) remains unclear. These fascinating results warrant further systematic study.

J. Tersoff
 IBM Research Division
 T. J. Watson Research Center
 P.O. Box 218
 Yorktown Heights, NY 10598

Received 24 September 1997 [S0031-9007(98)05443-X]
 PACS numbers: 68.35.Bs, 61.16.Ch, 68.35.Md

- [1] P. Hanesch and E. Bertel, Phys. Rev. Lett. **79**, 1523 (1997).
- [2] J. Tersoff and R. M. Tromp, Phys. Rev. Lett. **70**, 2782 (1993).
- [3] J. Tersoff, Phys. Rev. Lett. **74**, 4962 (1995).
- [4] J. Tersoff, Y. H. Phang, Z. Zhang, and M. G. Lagally, Phys. Rev. Lett. **75**, 2730 (1995).
- [5] F. Liu, J. Tersoff, and M. G. Lagally, Phys. Rev. Lett. **80**, 1268 (1998).
- [6] V. I. Marchenko and A. Ya. Parshin, Sov. Phys. JETP **52**, 129 (1980); V. I. Marchenko, JETP Lett. **33**, 381 (1981). See also, J. H. der Merwe and G. J. Shiflet, Surf. Sci. **256**, 171 (1991).
- [7] V. I. Marchenko, Sov. Phys. JETP **54**, 605 (1981).