

Step Energies and Roughening of Strained Layers

Recently Xie *et al.* [1] reported the fascinating and important result that the roughness of a strained layer depends sensitively on the sign of the strain. They noted that, because the steps on SiGe(001) have tensile stress, their formation energy is lowered by compressive strain but raised by tensile strain. The change in roughness was then attributed to the altered step formation energy. I wish to comment on two aspects of this interpretation.

First, strain-induced roughening of SiGe(001) typically takes the form of faceting, initially with (105) orientation [2,3]. Presumably such roughening is thermally activated [4]. Islands or pits of various sizes appear as thermal fluctuations, but they survive and grow only if they are larger than the critical size, i.e., the size with the most unfavorable energy. When the activation barrier is substantial, the rate of nucleation depends almost entirely on the energy of this “critical nucleus.”

Small thermal fluctuations no doubt consist of concentric step loops, but beyond some size a faceted shape is more favorable. Facets such as (105) have no simple connection to the steps studied in Ref. [1]. If the critical nucleus corresponds to a size where faceting has already set in, then the step energies have no direct relevance to the rate of roughening.

Instead, the activation barrier then depends upon the (105) and (001) surface energies [4]. Any change in the magnitude or *sign* of the strain will change these surface energies. (The change of surface energy with strain defines the surface stress.) Thus changing the sign of the strain will change the activation barrier, with an exponentially large effect on the rate of roughening. This is similar in spirit but not in detail to the interpretation suggested by Xie *et al.* and seems an equally plausible explanation for their observations.

The second point is that, while Xie *et al.* have added to our understanding of the step energetics, the picture is not yet complete. At a step on a strained layer, there is a discontinuity in the thickness and, hence, in the projected two-dimensional stress, creating a “force monopole” [5]. However, the effect is quite different than the force monopoles which have been previously considered [6,7], because the sign need not alternate for successive steps. The elastic relaxation which drives roughening is *entirely contained in the interaction of these monopoles*. Thus the step energy cannot be disentangled from the relaxation.

For simplicity, I describe the case without surface stress domains, e.g., for D_B steps. The total energy (per unit length parallel to the steps) to form steps at positions x_i may be approximated [7] as

$$E = \sum_i C_0 + \sum_{i \neq j} C_1 s_i s_j \ln \left(\frac{x_i - x_j}{a} \right) + \sum_{i \neq j} C_2 \left(\frac{x_i - x_j}{a} \right)^{-2}.$$

Here s_i is +1 for up steps and -1 for down steps; a is any convenient unit of length, e.g., the cell size; and

C_0 , C_1 , and C_2 are system-dependent constants. C_1 is proportional to (strain \times step height)², so this term is absent in the case of an unstrained layer.

Because of the long range of the logarithmic term, the energy of a step depends on the arrangement of distant steps—not only on their position, but also on whether they are up or down. As step pairs are created on a flat surface, the most favorable arrangement consists of all up steps followed by all down steps, or vice versa, forming a hillock or pit.

The incremental energy to add a step pair with a modest terrace width is probably positive at first (although absolute step energies are not reliably known), but the energy eventually becomes negative as the hillock or pit grows, due to the monopole interactions. Thus it seems likely that roughening is thermally activated in the stepped case, as in the faceted case. The absolute energies of steps arranged as in Ref. [1] then would not play a direct role in the roughening process. Still, the main point of Xie *et al.* is the lowering of C_0 under compression, and this remains crucial. A reduction of C_0 lowers the activation energy and so exponentially speeds the roughening process.

These points do not diminish the importance of the observations of Xie *et al.* or their insight in recognizing that step (or surface) stress will couple to the layer strain. However, for SiGe(001) a description in terms of faceting may prove more appropriate than one based on distinct steps. For systems where roughening does take place by step formation, the qualitative point of Ref. [1] is convincing, but a quantitative treatment requires recognition of the force monopole and associated logarithmic interaction, which arises at *any* step on a strained layer.

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