Morphological Evolution of Strained Films by Cooperative Nucleation

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We identify a new mechanism of stress driven surface morphological evolution in strained semiconductor films. Surface roughness forms by a cooperative mechanism involving the sequential nucleation of islands and pits, which is distinct from the conventional view of ripple formation as an Asaro-Tiller-Grinfeld (ATG) instability. This mechanism is operative both during annealing and growth and competes with the ATG instability as a kinetic pathway to ripple formation. [S0031-9007(96)00853-8]

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The morphological stability of stressed solids is a subject of considerable scientific and technological importance. It is directly relevant to several key issues in materials science ranging from stress corrosion cracking through to phase transformations and strained layer epitaxy. Since the pioneering work of Asaro and Tiller [1] and Grinfeld (ATG) [2], it is generally argued that above a critical wavelength λ_c the planar surface of a stressed solid is unstable to the formation of undulations [3–5]. This is because the energy reduction associated with elastic relaxation of the undulations exceeds the increase in surface energy. In the case of thin-film deposition, it is therefore envisioned that an initially planar film surface will gradually roughen in the growth direction over extended regions with a characteristic lateral wavelength. The observation of continuous surface ripple patterns on strained semiconductor layers over large areas would appear to give direct confirmation of this view [6,7]. Indeed, the patterns observed in cross section often closely resemble the sinusoidal roughness profiles used as a basis for the instability theory [8,9].

In this Letter we reveal an entirely new mechanism of surface ripple formation, which is linked to the activated nature of island and pit formation. The ripple forms by a cooperative mechanism involving the sequential nucleation of islands and pits. This is very different from the gradual strain induced roughening mechanism normally envisioned [3–9] and has important implications for our fundamental understanding of the 2D to 3D transition of strained systems.

To determine the mechanism of surface ripple formation we have studied the stress induced 2D to 3D transition in the technologically important Si_xGe_{1-x} system. Our method involves a novel two stage process in which a thin (5 nm) planar $Si_{0.5}Ge_{0.5}$ alloy layer is first grown at relatively low temperatures to ensure a nominally planar surface. The ripple morphology is then formed by a gentle postdeposition anneal at around 590 °C for 5 min. This approach emulates equilibrium surface conditions, at least locally, as closely as possible. A map of the surface evolution during growth was obtained from atomic force microscopy (AFM) measurements of the ripple geometry at different temperature regions of one sample wafer.

To capture the mechanism of surface ripple formation, use was made of the natural temperature gradient across the sample [10]. At the center of the wafer, corresponding to a temperature of 590 °C, a well-defined and continuous ripple geometry was observed using AFM as shown in Fig. 1(a). However, close to the edge region at 570 °C, isolated ripple domains consisting of alternating islands and pits were seen to be separated by planar regions of the strained layer [Fig. 1(b)]. This directly captures the transformation of a planar film to a ripple morphology. The continuous ripple in Fig. 1(a) is, therefore, just the coalesced stage of a cooperative nucleation process involving islands and pits. This is very different from the conventional ATG picture involving the simultaneous evolution of vertical roughness over large extended regions [3–9].

We now consider the physical origin of this cooperative nucleation mechanism of roughening. An isolated island (or pit) above a critical size will lower the energy of the planar strained film. However, to nucleate an island or pit it is first necessary to overcome an energy barrier [11]. Since the elastic interaction between islands and pits is negative (i.e., they attract), it is conceivable that cooperative effects may play an important role by lowering the activation barrier for domain growth. We therefore consider two possibilities of cooperative nucleation. The first possibility involves simultaneous nucleation in which an array of islands and pits form concurrently [12]. The second mechanism involves sequential nucleation where an island or pit nucleates adjacent to a preexisting stable configuration of islands and pits.

To examine these possibilities we consider a simple 2D model for domain growth which captures the essential physics of cooperative nucleation. Figure 2 shows several nucleation configurations involving various combinations of islands and pits. The nucleation of an individual island

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