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"Semiconductor Multilayers"

"Misfit Dislocations in Strained Layer Epitaxy: II. Kinetics" (Part IV)

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VIEWPOINT SET No. 19

MISFIT DISLOCATIONS IN STRAINED LAYER EPITAXY: II. KINETICS

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Introduction

In a companion paper (1), we summarized the energetic factors relevant to stress relaxation by misfit dislocations in strained layer epitaxy. In this paper, we discuss the kinetic factors relevant to strain relaxation rates. The rate at which a strained system will approach the equilibrium configuration predicted by equations (1) to (3) of Reference (1) will depend upon kinetic factors governing the nucleation, propagation and interaction of misfit dislocations. Here, we concentrate on the physics governing misfit dislocation motion, as the processes governing misfit dislocation nucleation and interactions are discussed in other papers by Hirth and Freund in this volume. The primary technique we have used to study misfit dislocation propagation is in-situ strained layer relaxation experiments in a transmission electron microscope (TEM) (2,3).

The amount of strain relaxation for a given area of lattice- mismatched interface will be governed by the equation:

$$L(t) = \int N(\sigma,t)\,v(\sigma,t)\,dt \quad - (1)$$

where $L(t)$ is the total length of interfacial misfit dislocation at time t, $N(\sigma,t)$ is the number of growing dislocations at time t and stress σ and $v(\sigma,t)$ is the propagation velocity of threading dislocations at (σ,t). The limits of this integral are from the start to finish of a post-growth annealing cycle (i.e. at constant epilayer thickness, h) or from the time at which the MB critical thickness is reached to final substrate cooling during a growth cycle. In (4) we discuss the detailed derivation of $N(\sigma,t)$, but in the present manuscript we discuss the theoretical modeling and experimental measurement of $v(\sigma,t)$. Given that eqn. (1) predicts a linear dependence of strain relaxation rate upon dislocation velocity, a detailed understanding of $v(\sigma,t)$ is clearly of great importance.

The Hirth–Lothe Diffusive Double Kink Theory

We have made extensive measurements of misfit dislocation propagation velocities by real-time in-situ observations of propagating dislocations during annealing of strained layer structures in a TEM (2,3). Experimental details are fully discussed in (3). A strength of these observations is that several measurements at different temperatures can be made *on the same dislocation*, thereby yielding accurate activation energies. We have observed markedly different apparent activation energies in the regimes of low interfacial dislocation density (dislocations moving essentially independently of each others' strain fields) and high dislocation density (dislocation motion strongly influenced by interactions with other defects). We denote these regimes as *non-interacting* and *interacting*, respectively. In this manuscript, we concentrate upon the non-interacting regime, where extrapolation should be possible to measurements of dislocation velocities made in bulk Si and Ge (e.g. 5-7).

In reference (3), we describe our attempts to reconcile our dislocation velocity measurements for Ge_xSi_{1-x}/Si(100) structures with the predictions of the Hirth-Lothe diffusive double kink model (8). In this model, a dislocation propagates by nucleation and motion of atomic-length segments of dislocation ("kinks") which lie transverse to the general dislocation line direction, as illustrated schematically in Figure 1. Geometrically, these kinks have to form in pairs in bulk materials. Kinks would also have to form in pairs in the configuration of a propagating threading arm in a buried strained epitaxial layer, but for uncapped epitaxial layers we have considered the possibility of single kink nucleation at the free surface (3).

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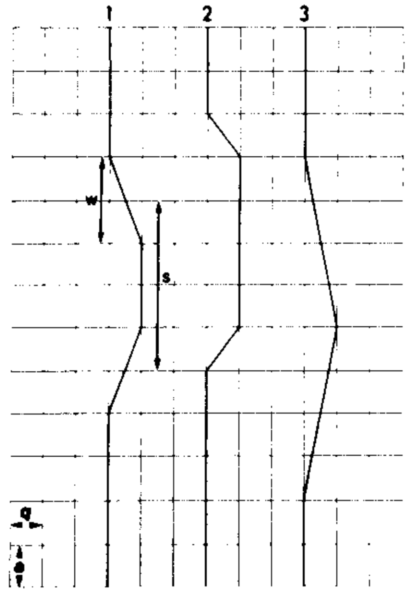

Figure 1: Schematic illustration of the double kink geometry showing double kink width, w, and separation, s. The predictions of the double kink model will be most accurate in the limits where kinks are well separated (examples 1 or 2) as opposed to overlapping (example 3). In this illustration the dislocations will propagate to the right by vertical motion of the kink pairs.

The diffusive double kink model predicts for the velocity of the propagating threading arm:

$$v = \frac{2\nu_D abq^2\sigma_{ex}}{kT} e^{\frac{-F'_k+E_m}{kT}} \frac{L}{L+X} \quad - (2)$$

Here, σ_{ex} is the "excess stress" driving dislocation motion, as described by Matthews-Blakeslee (9) and Dodson-Tsao (10) and derived in equations (1)-(3) of reference (1), ν_D is an attempt frequency for kink nucleation (which we approximate by the Debye frequency), q is the distance between Peierls valleys, b is the magnitude of the dislocation Burgers vector, a is the kink jump distance, $2F'_k$ is the energy required to nucleate a double kink, E_m is the energy barrier for kink jumps along the threading line direction, L is the length of the propagating threading arm and X is the average distance between double kinks given by:

$$X = 2ae^{\frac{F'_k}{kT}} \quad - (3)$$

The quantity F'_k may be modified by the applied stress, as first described by Seeger and Schiller (10):

$$2F'_k = 2F_{k0} - [\frac{G(1+\nu)\sigma_a b^3 q^3}{(1-\nu)kT}]^{1/2} \quad - (4)$$

where F_{k0} is the limit of F'_k at zero applied stress. This correction only becomes significant at applied stresses of the order hundreds of MPa or greater, which are generally not approached in bulk experiments but which may easily be exceeded in the strained thin films under study here. The Seeger-Schiller correction should be regarded only as approximate: it will work best at intermediate stresses in the hundreds of MPa range, but when σ_a approaches a GPa or more, the effect of overlapping kink arms (i.e. 2w < s in Figure 1) will render equation (4) invalid.

The limits of eqn. (2) are (i) L >> X, where kinks generally run into each other before reaching the end of the propagating dislocation. In this case, which is generally assumed for bulk materials, the numerator of the exponential becomes $(F'_k + E_m)$ and the ratio L/(L+X) disappears. (ii) L << X, where kinks generally reach the end of the propagating dislocation before annihilating each other. In this case, which may well be approached for thin epitaxial films, the exponential numerator becomes $(2F'_k + E_m)$ and the ratio L/(L+X) tends to L.

The diffusive double kink model, although generally invoked for dislocation motion in semiconductors, does not provide good quantitative agreement with measurements of dislocation velocity in bulk semiconductors. For Si and Ge, for example, the prefactors obtained from experiment are about two-three orders of magnitude higher than predicted by equation (2). This may be due to uncertainties in estimating the attempt frequency (although it is difficult to physically understand how this could be orders of magnitude higher than the Debye frequency!), or to obstacles to motion (constrictions, point defects etc.) along the dislocation line (at first sight these would appear to slow the experimental velocity with respect to theoretical prediction, but if they, for example, affected the experimentally determined activation energy, they could bring the prefactor into error).

Experimental Observations

We have been able to reconcile the Hirth-Lothe diffusive double kink model with our experimental observations (3) of dislocation velocities in Ge_xSi_{1-x}/Si(100) layers with x in the range 0.10 < x < 0.25 by (i) incorporating the Seeger-Schiller correction, eqn. (4), (ii) modeling single kink nucleation at the surface of thin uncapped epilayers and (iii) assuming a value of F_{k0} = 1.0 eV (which is intermediate to the range of available estimates of this quantity for Si in the literature). The overall dislocation glide activation energies we measure are consistent in the limit of low applied stresses with the values of ~ 1.6 eV and ~ 2.2 eV obtained for bulk Ge and Si respectively (e.g. 5-7). For x greater than about 0.25-0.30, the velocities we measure are lower than the Hirth-Lothe/ Seeger-Schiller predictions because eqn. (4) over-estimates the lowering of the kink nucleation energy. Examples of experimental measurement and theoretical modeling of dislocation velocities in capped Ge_xSi_{1-x} layers are shown in Figure 2.

Other measurements of dislocation velocities in Ge_xSi_{1-x}/Si(100) heterostructures have been made (12-14), and in general similar absolute velocities are obtained from measurements by different groups, see Figure 3. Tuppen and Gibbings (12) were able to model their data for dislocation velocities in thin capped Ge_xSi_{1-x} layers by assuming a dependence of dislocation velocity upon the length of the propagating threading arm, consistent with eqn. (2) in the regime where the epilayer thickness approaches, or is less than, X. The expected accompanying increase in activation energy was not, however, observed.

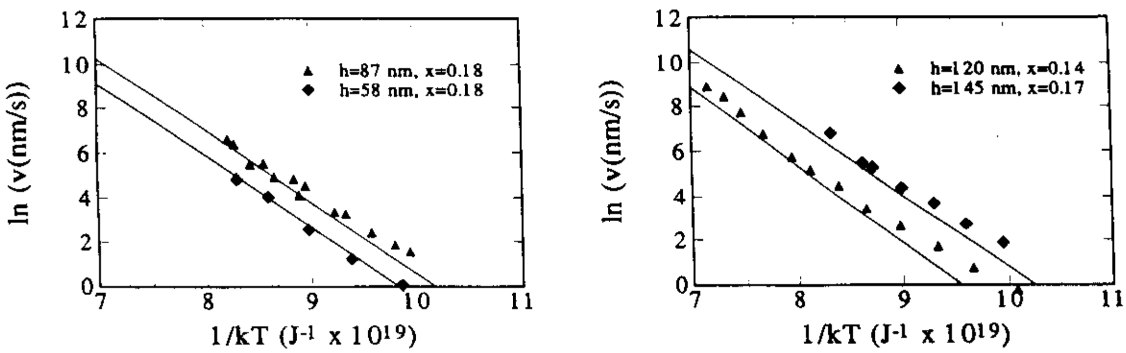

Figure 2: Measured dislocation velocities, v in $nm.s^{-1}$, for different Ge_xSi_{1-x} layers (x and epilayer thickness, h, given in legends) buried beneath 300 nm Si caps. The solid lines show the predictions of the Hirth-Lothe diffusive double kink model, with F_{k0} = 1.0 eV and incorporating the Seeger-Schiller correction, equation (4).

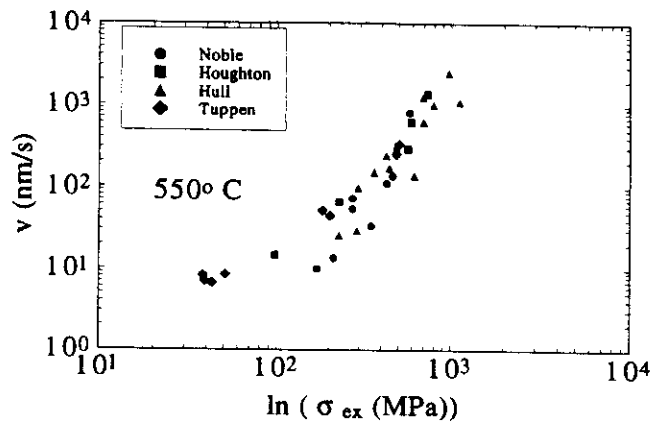

Figure 3: Misfit dislocation propagation velocities measured in (Si)/$Ge_x Si_{1-x}$/Si(100) as a function of excess stress. Velocities are interpolated from experimental data to a temperature of 550°C. Data are from references by Hull et al (3), Tuppen and Gibbings (11), Houghton (12) and Nix, Noble and Turlo (13).

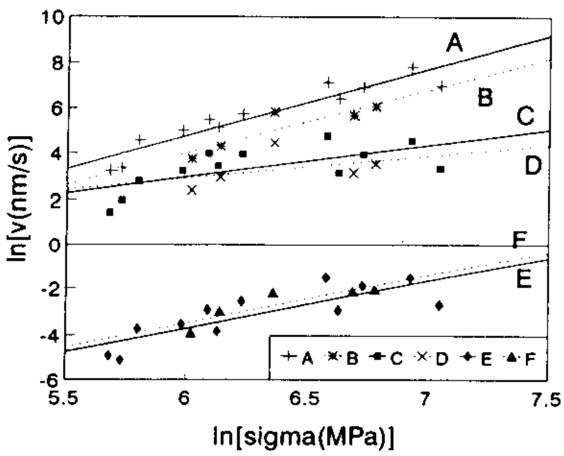

Figure 4: Variation of measured dislocation velocities at 550°C (v in $nm.s^{-1}$) vs excess stress (σ in MPa) for dislocations at $Ge_x Si_{1-x}$/Si(100) and (110) interfaces. Curves A and B correspond to raw velocity data for (100) and (110) structures respectively. Curves C and D correspond to (100) and (110) data respectively, with velocities normalized to the activation energy for motion in Si (by reducing the raw velocities for $Ge_x Si_{1-x}$ in curves A and B by exp[0.6x(eV)/kT]). Curves E and F correspond to curves C and D respectively, but now further normalized by the length of the propagating threading arm lengths, L.

We show in Figure 4 an investigation of the effects of stress and propagating dislocation length upon dislocation velocity for structures grown upon (100) and (110) surfaces. In curves A and B, we show the variation of ln(v) with ln(σ_{ex}). The trend of increasing v with increasing σ_{ex} is evident. Note that the gradient, m=2.9, of the interpolation lines implies a significantly greater than linear dependence of velocity upon excess stress in the prefactor of eqn. (2). A similar effect has been previously pointed out by Houghton (13), who observed that m~2, but we believe this non-linear dependence upon excess stress to be at least partially due to the general increase in Ge concentration (x in $Ge_x Si_{1-x}$) for the higher excess stress films. The lower glide activation energy of Ge with respect to Si then increases the velocities in these higher stress films. If the data points for the (100) and (110) surfaces are normalized to the same activation energy, the average gradients of the interpolation line become close to 1 at m=1.2, as shown in curves C and D of Figure 4. The correlation coefficient for the curves C and D, however, is relatively low at an average of 0.54. In curves E and F, we show the results for dislocation velocities which have both been normalized by a compositionally-dependent activation energy (as in curves C and D) and by the lengths of the propagating dislocation arms (in general for these structures we are in a regime L<<X, so we expect v to be approximately proportional to L as discussed above). A much more satisfactory average correlation coefficient of 0.85 is now observed. The interpolation line gradients now increase to an average m=2.0. This apparent super-linear dependence upon excess stress is probably due to the lowering of the kink nucleation energy by higher applied stresses, predicted by the Seeger-Schiller factor.

The precise details of the kink nucleation energies and diffusive kink regimes (relative magnitudes of L and X) make very substantial differences in dislocation velocities and strain relaxation rates. For example, consider capped $Ge_x Si_{1-x}$ layers 100 nm thick grown on Si(100) with compositions x=0.15 and x=0.20. If the only difference in velocity is due to a linear prefactor dependence upon excess stress, the ratio of velocities in the two structures would be 1.3. Incorporating the change in activation energy with Ge composition (linearly interpolating between 1.6 eV for Ge and 2.2 eV for Si) produces a velocity ratio of about 4. Calculation from the full Hirth-Lothe formula, including the Seeger-Schiller correction, would produce a velocity ratio of about 20. Comparison of experimental data from two actual structures which approximate these hypothetical structures (120 nm x=0.14 and 100 nm of x=0.20), yields a velocity ratio of about 8 (3), which is intermediate between these predictions. This underlines the substantial increase in instability to strain relaxation with increasing composition in $Ge_x Si_{1-x}$/Si heterostructures.

Conclusions

We have discussed the physical mechanisms governing propagation of misfit dislocations in $Ge_x Si_{1-x}$/Si heterostructures. Predictions of dislocation propagation velocities, which are central to determining strain relaxation kinetics, are complex when based upon the Hirth-Lothe diffusive double kink model. Reasonable agreement between experimental measurement and diffusive kink theory (including the Seeger-Schiller correction for stress-induced lowering of the kink nucleation energy) can be obtained for $0.10 < x < 0.25$ in $Ge_x Si_{1-x}$/Si(100) with a derived value of F_{k0} = 1.0 eV. Comparison of dislocation velocities with different applied stresses suggests that the stress-induced glide activation energy reduction, although present, is somewhat less than predicted by the Seeger-Schiller formula.

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