Abstract
Metamorphic semiconductor devices use compositionally-graded buffer layers for accommodation of lattice mismatch with controlled dislocations and strain. Linearly-graded buffers have been used extensively, but there are indications that sublinear, superlinear, S-graded, or overshoot graded structures could offer advantages. We compared linear and nonlinear grading approaches for \( \text{InGaAs}_x \text{As} \) grown on GaAs (001) substrates in terms of dislocation density profiles using a dislocation dynamics model.

Introduction
Graded layers are used to accommodate lattice mismatch in semiconductor devices to control the dislocation density. The surface threading dislocation density decreases with total material thickness but is also influenced by the profile of grading, and it is desirable to use the minimum buffer thickness. It is believed that dislocation interactions, especially pinning interactions such as those shown in figure 1, influence the performance of graded buffers, but until now models for this behavior have been limited so most studies have been empirical. Here we use a dislocation dynamics model with pinning interactions included to compare grading approaches in \( \text{InGaAs}_x \text{As}/ \text{GaAs} \) (001) graded layers.

Dislocation Dynamics Model
In a semiconductor heterostructure the rate of relaxation \( \gamma(z) \) at a distance \( z \) from the interface is [1]

\[
\frac{d\gamma(z)}{dt} = KBb \sin \alpha \cos \lambda \sigma_{\text{eff}}^2(z) \exp \left( \frac{\gamma}{\kappa} \right) \int_0^\infty \rho_A(\gamma) \, d\gamma + \rho_0 \delta(\gamma),
\]

where \( \alpha \) is the angle between the Burgers vector and line vector, \( \lambda \) is the angle between the Burgers vector and the line in the interface plane which is perpendicular to the intersection of the glide plane and the interface, \( \sigma_{\text{eff}}(z) \) is the effective stress, \( U \) is the activation energy for dislocation glide, \( k \) is the Boltzmann constant, \( T \) is the temperature, \( \rho_A(\gamma) \) is the cross-sectional density of misfit dislocations, and \( \rho_0 \) represents an initial density of defects, and \( B \) and \( K \) are semi-empirical constants. For \( \text{InGaAs}_x \text{As} \), \( B = (0.48 + x1.74 - x^20.42) \times 10^{-3} \, \text{cm}^3 \, \text{dyne}^{-1} \, \text{s}^{-1} \), and \( U = \{1.3 + 0.1x\} \, eV \).

The effective stress is

\[
\sigma_{\text{eff}}(z) = \left( \frac{2Kb \cos \alpha}{Kb} \right) \int_0^z \left( \frac{\gamma_{\text{crit}}(z') - \gamma(z')}{(1 + \gamma(z'))^{1/2}} \right) \, dz',
\]

where \( \phi \) is the angle between the surface normal and the slip plane, \( v \) is the Poisson ratio, \( \epsilon(z) \) is the in-plane strain at a distance \( z \) from the interface, \( \epsilon_{\text{eq}}(z) \) is the equilibrium in-plane strain, and \( \zeta \) is a variable of integration. The areal density of misfit dislocations is

\[
\rho_A(z) = \left( \frac{1}{b \sin \alpha \cos \lambda} \right) \frac{\partial \gamma}{\partial z} + \frac{\partial \rho_0(\gamma)}{\partial z}.
\]

The length of misfit dislocations \( L_{MD} \) is given by

\[
L_{MD} = \int_{\gamma_0}^\infty 2B \sigma_{\text{eff}} \exp \left( \frac{\gamma}{\kappa} \right) \, d\gamma,
\]

where \( \gamma_0 \) represents the time of onset of lattice relaxation, corresponding to the critical layer thickness, and \( \gamma \) is a variable of integration. The threading dislocation density \( D \) is found by

\[
D(z) = \frac{4\rho A(z)}{\sin \alpha \cos \lambda} \frac{\partial \rho A(z)}{\partial z} = \frac{L_{MD}(z)}{2B \sigma_{\text{eff}}(z)},
\]

where \( L_{MD}(z) \) is the average length of misfit segments, and \( L_{MD}(z) \) is the interaction length for annihilation and coalescence reactions. We assume a dislocation will become pinned if it glides within the pinning radius of an orthogonal dislocation as shown in figure 2. Then the maximum length of misfit dislocations may be estimated as

\[
L_{MD,\text{max}}(\zeta) = \left( \frac{\int_{\gamma_0}^{\max} \rho_A(\gamma) \, d\gamma}{\gamma_0} \right)^{1/2},
\]

where \( \zeta \) is a variable of integration, and the pinning radius is

\[
\gamma_0 = \sqrt{2kBb} / 2\pi \sigma_{\text{eff}} \cos \lambda.
\]

Results
We compared sublinear, linear, and superlinear buffer layers of \( \text{InGaAs}_x \text{As} \) grown on GaAs (001) substrates at 510°C with a growth rate of 0.5 μm/hr. The compositional profiles of these “gamma-graded” layers were generated using the universal equation \( x = x_{\text{top}} \left( \frac{z}{L} \right)^n \), where \( y \) is the top composition, \( h \) is the layer thickness, and the parameter \( \gamma \) determines the nature of the profile; values less than one result in sublinearity, values greater than one result in superlinearity, and a value of one corresponds to linear grading. Figure 3 shows the compositional profiles for \( \gamma \)-graded \( \text{InGaAs}_x \text{As} / \text{GaAs} \) (001) layers having a thickness of 0.5 μm and a top indium composition of 0.25. Figure 4 shows the resulting misfit dislocation density profiles. Lower values of \( y \) concentrate the misfit dislocations near the interface while higher values of \( y \) skew the misfit dislocation density toward the top surface. Figure 5 illustrates the associated threading dislocation densities. The surface threading dislocation density varies considerably with the value of \( y \). Although it is generally considered better to avoid concentrations of misfit dislocations, due to pinning interactions, concentration of misfit dislocations near the interface is less harmful than concentration at the surface, so that the surface threading dislocation density varies monotonically with gamma.

Conclusion
We have applied a dislocation dynamics model, extended to include dislocation pinning interactions, to compare the performance of sublinear, linear, and superlinear graded layers of \( \text{InGaAs}_x \text{As} \) on GaAs (001) substrates. This model is applicable to the further study of general graded and multilayered heterostructures.