A Zagging and Weaving Model for Dislocation Interactions in Heterostructures Containing Strain Reversals

Tedi Kujofsa¹ and John E. Ayers¹,²

¹Electrical and Computer Engineering Department, University of Connecticut, Storrs, CT 06269 USA
²Epitax Engineering, Ashford, CT 06278 USA

Abstract

Strained-layer superlattices (SLSs) have been used to modify the threading dislocation behavior in metamorphic semiconductor device structures; in some cases they have even been used to block the propagation of threading dislocations and are referred to in these applications as “dislocation filters.” However, such applications of SLSs have been impeded by the lack of detailed physical models. Here we present a “zagging and weaving” model for dislocation interactions in multilayers and strained-layer superlattices, and we demonstrate the use of this model to the threading dislocation dynamics in InGaAs/GaAs (001) structures containing SLSs.

Motivation

Strained-layer superlattice (SLS) structures are used to reduce the dislocation density and improve performance in semiconductor devices (see fig. 1), and these are occasionally referred to as “dislocation filters.” However, use of SLSs in this way has been hindered by the need for empirical design, and we therefore sought to extend the standard dislocation dynamics model to include zagging and weaving for application to SLSs and other multilayered structures.

Model for Lattice Relaxation

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

$$\frac{d\gamma(z)}{dt} = KBh \sin \alpha \sigma_{eff}(z) \exp \left( -\frac{U}{kT} \right) \int_0^\beta \rho_0 \alpha d\zeta ,$$

[1]

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, $\sigma_{eff}(z)$ is the effective stress, $U$ is the activation energy for dislocation glide, $k$ is the Boltzmann constant, $T$ is the temperature, $\rho_0(\zeta)$ is the cross-sectional density of misfit dislocations, $\rho_1$ represents an initial density of defects, and $B$ and $K$ are semi-empirical constants.

For In$_{0.3}$Ga$_{0.7}$As, $B = (0.48 + x1.74 - x^20.42) \times 10^{-6} \text{ cm} \text{ dy}^{-1}, K = (0.33 + x23 - x^20.41) \times 10^{-6} \text{ cm} \text{ dy}^{-1}, \text{ and } U = 1.3 + 0.1x eV$ [2]. The effective stress is

$$\sigma_{eff}(z) = \frac{2K\sigma x \cos \alpha}{(1 + \nu)} \int_0^\beta \left\{ \gamma - \gamma_0 \right\} d\zeta ,$$

[2]

where $\phi$ is the angle between the surface normal and the slip plane, $\nu$ is the Poisson ratio, $\epsilon(z)$ is the in-plane strain at a distance $z$ from the interface, $\epsilon_0(z)$ is the equilibrium in-plane strain, and $\xi$ is a variable of integration. The areal density of misfit dislocations is

$$\rho_0(z) = \frac{1}{(1 + \alpha^2 \cos^2 \alpha)} \left( \frac{\alpha}{\beta} \right) .$$

[3]

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

$$L_{MD}(z) = \int_0^\beta 2B_\sigma_{eff} \exp \left( -\frac{U}{K} \right) d\zeta ,$$

[4]

where $\tau_0$ represents the time of the onset of lattice relaxation, corresponding to the critical layer thickness, and $\tau$ is a variable of integration. The equation governing the variation of the threading dislocation density $D$ is

$$\frac{dD(z)}{dz} = 4\pi \rho_0(z) / L_{MD}(z) \sin \beta \rho_0(\zeta) - L_{11}(z) D^2(z) ,$$

[5]

where $\rho_0(z)$ is the cross-sectional density of misfit dislocations, $L_{MD}(z)$ is the average length of misfit dislocation segments, and $L_{11}(z)$ is the interaction length for annihilation and coalescence reactions between threading dislocations. Here we account for the zagging and weaving of dislocations at mismatched interfaces so the interaction length accumulates with the total length of a jogging dislocation such as that shown in figure 2. Therefore

$$L_{11}(z) = \int_0^\beta \cos \alpha \left( \begin{array}{c} \sigma \left( L_{MD}(\zeta) \right) \end{array} \right) d\zeta ,$$

[6]

where $\beta$ is the angle between the slip plane and the interface.

Results

To investigate the effect of inserting a superlattice in an InGaAs/GaAs (001) structure, we considered four heterostructures grown at 510°C with a growth rate of 0.5 μm/hr. Using a SLS design comprising five periods of 10-nm In$_{0.3}$Ga$_{0.7}$As/10-nm In$_{0.5}$Ga$_{0.5}$As, we found the threading dislocation density profiles for four cases having a superlattice at the interface, midway through a uniform layer, and at the top, as well as the case of no SLS. The uniform material was In$_{0.3}$Ga$_{0.7}$As with a total thickness of 1000 nm. The results in figure 3 show that the structure without an SLS contains $1.5 \times 10^{10}$ cm$^{-2}$ dislocations but insertion of SLS at the interface decreases the dislocation density to $0.37 \times 10^{8}$ cm$^{-2}$. Inserting the SLS farther from the interface actually increases the surface dislocation density.

Next we considered the strength of the superlattice, varying the step in the composition and comparing to the case of no SLS as shown in figure 4. The temperature, growth rate, and total thickness of uniform material was the same as before. While these results show a weak dependence on the compositional step used in the SLS, the best case is the one with the smallest compositional step, containing a five period 10-nm In$_{0.3}$Ga$_{0.7}$As/10-nm In$_{0.5}$Ga$_{0.5}$As superlattice.

Conclusion

The dislocation dynamics model described here, extended to account for zagging and weaving in multilayered structures, predicts the dislocation filtering property of superlattices and will be applicable to the design of device structures.