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A theoretical model for threading dislocation reduction during selective area growth

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Abstract

An analytic model, developed earlier for understanding the reduction kinetics of threading dislocations (TDs) in the heteroepitaxial growth of thin films, is considered here for the special case of selective area growth, wherein mesas of comparatively small lateral dimension are grown on a substrate. TD ensembles are treated in close analogy with chemical species in chemical reaction kinetics. In addition, a computer simulation approach that incorporates specific TD crystallography and considers the individual geometry of and reactions between TDs is used to augment the analytic results. The model is applied to three mesa geometries, encompassing squares as well as a rectangle. It is found that the density of TDs decays exponentially with increasing film growth, consistent with the enhanced reduction noted in several experimental reports. © 1997 Elsevier Science S.A.

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1. Introduction

In semiconductor fabrication, there is increasing drive to exploit material systems in which a film and substrate have large lattice mismatches. In the growth of lattice-mismatched epitaxial thin films, misfit dislocations (MDs) are concomitantly generated with threading dislocations (TDs). The former are equilibrium interfacial defects that inevitably form to accommodate the strain mismatch, while the latter link the MDs to the free surface and possess a negligible equilibrium density since they necessarily raise the energy of the film [1,2]. TDs are deleterious for physical performance of electronic devices, and there has been a substantial experimental effort to reduce their densities. Despite the large amount of research aimed at theoretically and experimentally understanding MD generation, there have been relatively few theoretical efforts [1–6] to understand the mechanisms by which TDs are eliminated.

Typically, for large mismatch films (e.g. mismatch strains in excess of $\sim 2\%$), TD densities are quite high near the film/substrate interface, often on the order of 10^{10}–10^{11} cm^{-2}. Several experimental studies on relaxed or nearly-relaxed films (for which the film thickness h greatly exceeds the critical thickness for MD formation) [1,7,8] have established that TD density is proportional to the inverse of the film thickness through the range of 10^{8}–10^{9} cm^{-2}. At lower densities, a weaker decay is observed. Romanov and coworkers [2–6] have formulated a model which is quantitatively consistent with experimental observations for homogeneous buffer layers—namely, it predicts the $1/h$ dependence of TD density as well as the saturation behavior. The latter comes about from long-range fluctuations in the net Burgers vector content of the local TDs [2].

Also, it is possible that TDs can propagate out of the growth area. If the lateral dimensions of the growing film are small enough, this effect may be significant (see Fig. 1). This use of mesas, or selective area growth, was first recognized by Matthews et al. [9] for its possible role in reducing TD densities. Other researchers, nota-

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bly Fitzgerald et al. [10–14], Knall et al. [15,16], and Yamaguchi [17] have provided data that shows TD (and MD) densities can be dramatically reduced by reducing the growth area. A common explanation for the reduced defect densities involves the altered stress state due to edge effects in the mesas and its subsequent role in driving defects towards edges or perhaps even suppressing dislocation nucleation sources. Although this may indeed be an important consideration in strained mesas, the theory presented here accounts for inherent migration of TDs towards the sidewalls, which may or may not be stress induced. The sidewalls act as an appreciable sink, and we believe this mechanism to be especially important in mesas that are formed as the extended growth of a pre-relaxed structure.

2. Analytic model

Previously, Romanov and coworkers [2–6] considered the possible mechanisms of TD reduction in a general framework which appeals to various sources of TD motion, specific TD reaction mechanisms that are connected with local forces between TD segments, and connects these reactions and motions with internal and external parameters such as the Peierls stress, temperature, misfit strain, film thickness, etc. In contrast with earlier treatments of the problem of TD reduction, this approach incorporated specific crystallography and geometry of TD migration and reactions in a quantitative fashion.

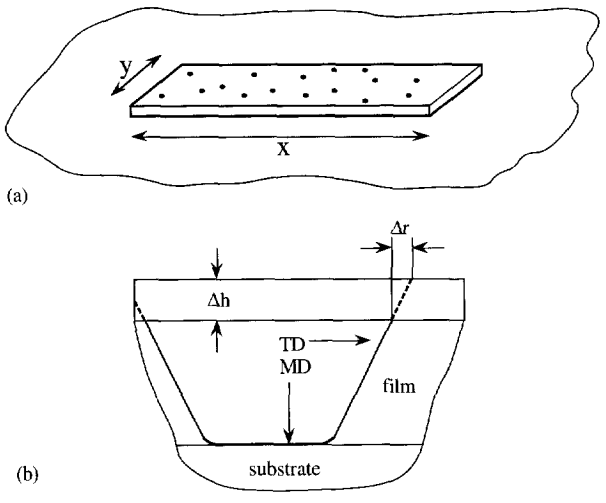

Fig. 1. (a) Schematic of an epitaxial mesa grown on a substrate, with dark points representing the intersection of threading dislocations with the film surface. The TDs merge into misfit dislocations lying on the mesa/substrate interface (not shown). (b) Effective motion of TDs in semiconductor epitaxy. Shown are idealized straight TD segments, one of which has undergone a change in position Δr due to the incremental growth of the film, Δh. Another has intercepted the mesa sidewall during the growth step and no longer participates in the reaction kinetics.

Relative TD motion may be achieved, for example, by changing layer thickness (e.g. growth of homogeneous buffer layers), by the strain-driven migration of TDs to generate MDs in strained layer growth, or by point defect condensation [3]. The TD motion r, which is defined as the lateral movement of the intersection point of the TD with the free surface, may be written in the form.

$$r = r(h, \epsilon_0, c) \tag{1}$$

where h is the film thickness, ϵ_0 is the misfit strain between the film and substrate, and c is the non-equilibrium point defect concentration in the film. The primary source of motion accounted for in the current work is the translation of TD intersection points with the film surface as it continuously grows (Fig. 1(b)). In general, r is not treated as a state variable.

Simultaneously, we assume reactions (associated with rapid processes) occur when the separation of TD pairs is less than a reaction radius, r_I. The reaction radius r_I represents the distance at which the interaction force between TDs is sufficient to overcome the Peierls barrier σ_p for TD glide or climb. Once initiated, this movement results in reaction and this is considered to be a fast process in comparison to motion, r. Romanov et al. [3] suggested the reaction radius has the following dependence

$$r_I = r_I(\sigma_p, T, t, c) \tag{2}$$

In Eq. (2), it is assumed that temperature T, time t, and point defect concentration c, can all contribute to the change of the reaction radii either through thermally-activated glide or point defect-assisted climb. Here, we assume a constant value of r_I.

The possible reactions between TDs include annihilation, fusion, and scattering [2]. In an annihilation reaction, TDs with opposite Burgers vectors that fall within an annihilation radius r_A react and stop the propagation of both TDs to the film surface. In a fusion reaction with a characteristic reaction radius r_F, two TDs react to produce a new TD with Burgers vector which is the sum of Burgers vectors of the reacting TDs. In a scattering reaction with a characteristic reaction radius r_S, the line direction and slip plane of one or both reacting TDs changes as a result of repulsive interactions.

The geometrical ideas discussed above prompted Romanov et al. [4] to describe TD density evolution for the specific case of a relaxed buffer layer with a finite lateral dimension, Λ, as might be realized in selective area growth over a relaxed layer with a high TD density. Both reactions between TDs and their disappearance through edges should be considered, in cases for which motion depends only on the thickness, h (see

Fig. 1). As a result, the change in TD density with film thickness may be written as [4]

$$\frac{d\rho}{dh} = -\frac{\rho}{\Lambda} - K\rho^2 \tag{3}$$

where $K = 2Gr_I$, and $G = dr/dh$ is a geometric factor that describes TD motion during film growth and commonly $G \approx 1$ for inclined TDs in (001) cubic semiconductor films. The development of Eq. (3) is discussed in more detail by Romanov et al. [3,4]. In this case, the terms on the right hand side of Eq. (3) are analogous to those usually used in first and second order reaction kinetics, respectively. Integration of Eq. (3) yields

$$\rho = \frac{\rho_0}{(1 + K\Lambda\rho_0)\exp\left(\frac{h - h_0}{\Lambda}\right) - K\Lambda\rho_0} \tag{4}$$

where ρ_0 is the TD density at the initial thickness h_0. In the limit of a large mesa size in comparison with the film thickness, $\Lambda \gg h - h_0$, the solution corresponds to that for homogeneous buffer layers, i.e.

$$\rho = \frac{1/K}{h + \hat{h}} \tag{5}$$

where $\hat{h} = (\rho_0 K)^{-1} - h_0$. This is in agreement with experimental observations of TD density in homogeneous buffers [7,8], and is the limiting situation studied by Romanov et al. [2–6].

The intentional use of selective area growth, i.e. use of films with small lateral dimensions (mesas), is now considered. It has been observed that TD reduction is efficient under these circumstances. We believe that our framework provides a ready explanation of this behavior, since TDs can readily grow out of the mesa laterally in a short time period. We may demonstrate this by considering Eq. (6) for the case where $\Lambda \to 0$, i.e. for the limiting case of small mesas:

$$\rho = \rho_0 \exp\left(-\frac{h - h_0}{\Lambda}\right) \tag{6}$$

Note that this gives exponential decay of TD density. Since we will present cases for the growth of a film from relatively small thickness ($h - h_0 \ll \Lambda$) through the regime where mesa size effects dominate ($h - h_0 \gg \Lambda$), we will use the more general form, Eq. (4), when showing specific results in Section 4 of this paper.

3. Computer simulation approach

The analytical treatment mentioned thus far is a mean-field approach; hence, it does not take into account spatial fluctuations in the densities of particular families of TDs. The generalization of the differential equations to include spatially varying TD densities is an extremely challenging mathematical problem; therefore, a computer simulation approach is a more viable alternative for understanding the spatial-dependent aspects of TD reduction. A simulation of the evolution of TD arrangements in growing films has been proposed by Beltz et al. [6], and is a variant of 2-D dislocation dynamics similar to those used for modeling of dislocations in bulk materials [18]. The idea of the simulation is to consider a domain (representing the film surface plane) with a given distribution of TDs and to investigate the evolution of the TD ensemble when each dislocation has a prescribed trajectory for motion and can react with another dislocation when their separation becomes smaller than a reaction radius. Dislocations may exit the domain of the simulation; however, a new dislocation of the same type is introduced at a random location on the opposite domain edge. This eliminates artificial loss of dislocations due to boundary effects. If we remove this random re-introduction of TDs, then the model becomes appropriate for small mesa growth. When modeling selective area growth, the simulation domain is considered to be the *entire* growth area, thus, there is no such re-introduction of TDs.

In the simulation results presented here, points representing TD intersections with a film surface were translated laterally as the films grows, according to prescribed TD trajectories in (001) oriented face centered cubic films. All pairs of TDs that fell within r_I were either removed (annihilation) or combined into a single TD (fusion). Specific details on the simulation procedure may be found in [6]. Specific results presented in this paper are for an r_I of 500 nm and mesa sidewalls parallel to $\langle 100 \rangle$ directions in the film material.

4. Results and concluding remarks

Three mesas are considered in this paper — two squares and one rectangle. The sizes are $200r_I \times 200r_I$, $200r_I \times 40r_I$, and $40r_I \times 40r_I$. These dimensions correspond to the lengths X and Y shown in Fig. 1(a). The simulation results to be shown are for a case in which all the initial TDs consist of equal populations of those with inclined Burgers vectors, and zero population of those with Burgers vectors parallel to the film/substrate interface. The particular choice of initial distribution is quite arbitrary here, and corresponds to a case in which the net Burgers vector content in the film is identically zero. Situations in which the initial net Burgers vector content is nonzero are very important when considering homogeneous buffer layer growth ($\Lambda \to \infty$), but do not seem to have an effect on the particular results that we show for selective area growth. Moreover, we considered cases for which the mesa sidewalls are oriented along $\langle 110 \rangle$ directions in the film, and this had minimal effects on the simulation results. These effects

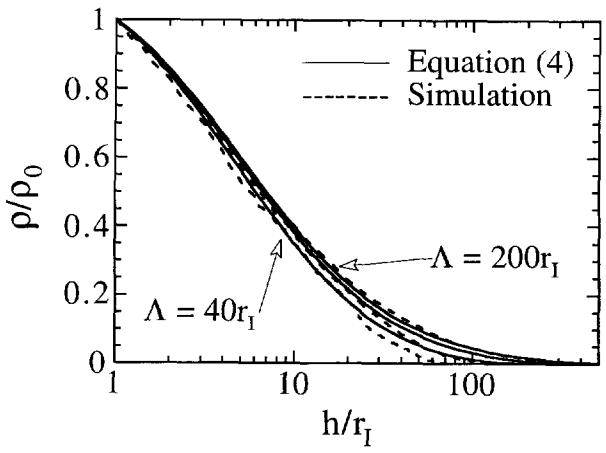

Fig. 2. The thickness dependence of TD density for selective area growth over a relaxed layer for mesa dimensions of $200r_I \times 200r_I$ ($\Lambda = 200r_I$), $200r_I \times 40r_I$ ($\Lambda = 89.44r_I$), and $40r_I \times 40r_I$ ($\Lambda = 40r_I$). For all cases, $\rho_0 K r_I = 0.16$ and the geometric factor G was taken as unity.

warrant further investigation in the context of selective area growth; however, we will limit our discussion here to the case with equal initial densities of TDs with inclined Burgers vectors, with sidewalls along $\langle 100 \rangle$ directions.

The thickness dependence of the total TD density ρ/ρ_0 is shown for the various cases in Fig. 2. For all three cases, the solid lines correspond to the analytic result, Eq. (4), with $\rho_0 K r_I$ taken as 0.16. The dashed lines correspond to the simulation results, which show remarkably close agreement with the analytic results. Note the rapid decay to zero TD density for increasing film thickness—an effect which is accelerated for smaller mesa sizes. Self consistent values of K and r_I must be used when making a valid comparison between the analytic and computational results; this relationship is identical for homogeneous buffer layers and is taken up in references [4,5]. Here, a more important issue concerns the value of Λ. The specific value chosen for Eq. (6) was the geometric mean of the mesa dimensions used in the simulation, i.e. $\Lambda = \sqrt{XY}$.

In summary, we have considered the general problem of the reduction in TD density during selective area growth of mismatched epitaxial films. The physical mechanisms responsible for TD reduction are reactions between TDs that lead to either annihilation or fusion, as well as TDs exiting through the mesas sidewalls. In the future, we will consider specific crystallographic effects via the computer simulation and analytic approaches, including the effects of initial TD distributions possessing zero and nonzero net Burgers vector contents.

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