

phys. stat. sol. (b) **198**, 599 (1996)

Subject classification: 61.72 and 68.55; S5.11; S5.12; S7.11; S7.12

*Arbeitsgruppe Mechanik Heterogener Festkörper, Max Planck Gesellschaft, Dresden*¹⁾ (a),
Materials Department (b) and Mechanical Engineering Department (c),
*University of California, Santa Barbara*²⁾

Modeling of Threading Dislocation Density Reduction in Heteroepitaxial Layers

I. Geometry and Crystallography

By

A. E. ROMANOV³⁾ (a), W. POMPE (a), G. BELTZ (b), and J. S. SPECK (c)

(Received July 15, 1996)

The geometry of threading dislocations (TDs), non-equilibrium defects that are generated as a result of stress relaxation in thin films, is considered in order to provide a basis for their reduction behavior during heteroepitaxial growth. This paper, the first of a two-part series, discusses the geometric possibility for reactions between TDs as a result of film growth. It is demonstrated that effective TD motion and reaction are responsible for their overall reduction. The reactions become possible if pairs of TDs come within a critical distance: r_A for annihilation reactions, r_F for fusion reactions, and r_S for scattering reactions. The model is used to explain the experimentally observed $1/h$ (h is the film thickness) dependence on TD density. The crystallographic consideration of TDs in the case of (001) growth of f.c.c. semiconductor films is presented and possible reactions between TDs in this case are analyzed.

1. Introduction

In the development of semiconductor devices, there is an increasing drive to utilize systems in which the film and substrate have large lattice mismatches. The need to work with large lattice mismatched systems is based both in technology and economics. For many systems, the need to control energy gap leads to alloy compositions that are not lattice matched to any commonly available single crystal semiconductor substrate; this is the case in common systems such as $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ (001) or $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ (001). Many substrates are unavailable in large areas because of limitations in growth technology. For example, CdTe and related compositions $\text{Cd}_{1-y}\text{Zn}_y\text{Te}$ cannot be grown as large single crystal boules. In many cases, the substrate material has such low fracture toughness that large area substrates are unviable. The difficulties and cost associated with bulk GaAs lead to the extensive and partially successful effort during the 1980s to develop GaAs on Si technology. Thus, the science and technology of lattice mismatched systems require further theoretical investigation [1]. In particular, theoretical investigations of misfit dislocations (MDs) and associated threading dislocations (TDs) that are essential elements of thin film systems must be developed.

¹⁾ Hallwachstr. 3, D-01069 Dresden, Germany.

²⁾ Santa Barbara, CA 93106, USA.

³⁾ Permanent address: A. F. Ioffe Physico-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia.

In Parts I and II of this paper we expand upon our previous theoretical work on TD reduction [2]. In Part I, we discuss the background on TD generation and then review experimental evidence for dislocation reduction in semiconductor buffer layers. We then provide a simplified basis for TD reduction. A general treatment involving inclined TDs is developed and applied to TDs in (001) f.c.c. films. Finally, geometrical arguments are presented for development of scaling laws for TD reduction. In Part II, a series of coupled differential equations is derived that describe the specific details of TD densities in homogeneous buffer layers. Solutions for a range of initial TD densities, applicable to different thin film growth modes, are obtained and discussed.

The model developed in Parts I and II is based on the crystal geometry of TD reactions and on the consequent TD “kinetics”. The analytic formalism includes the geometric cross-section for TD annihilation and fusion reactions. The solutions to the simplified equation and series of coupled differential equations show that the total TD density is inversely proportional to film thickness h , as experimentally observed. We find in Part II that the saturation behavior in TD density is due to finite local Burgers vector content.

2. Background

2.1 Misfit dislocation and threading dislocation generation

Misfit dislocation (MD) and threading dislocation (TD) generation must be considered for situations in which the film is grown well in excess of a critical thickness. For lattice mismatched films, regardless of the growth mechanisms, such as Frank-van der Merwe (layer-by-layer), Stranski-Krastanov (initial wetting followed by islanding), or Volmer-Weber (incoherent islanding) increasing film thickness will ultimately lead to MD generation and concomitant TDs. For either island mechanism, TDs may result from surface half-loop generation or from island coalescence.

For epitaxial systems in which the film wets the substrate, Frank-van der Merwe growth results. The mismatched film will grow strained but MD free until it reaches a kinetic critical thickness h_k in excess of the Matthews-Blakeslee critical thickness h_c , where h_c is given as

$$h_c = \frac{|\mathbf{b}|}{\varepsilon_m(1 + \nu) 8\pi \cos \lambda} (1 - \nu \cos^2 \beta) \ln \left(\frac{\alpha h_c}{|\mathbf{b}|} \right), \quad (1)$$

where ε_m is the misfit strain, ν is Poisson’s ratio, $|\mathbf{b}|$ is the magnitude of the Burgers vector of the dislocation, λ is the angle between $\mathbf{b}$ and a line perpendicular to the MD line that lies in the film/substrate interface, β is the angle between $\mathbf{b}$ and the dislocation tangent line, α describes both the core cut-off radius invoked in continuum mechanics approximations for strain energies of dislocations and the boundary condition at the film free surface [3].

For a fully relaxed film, the linear MD density $\varrho_{\text{MD, relaxed}}$ multiplied by the edge component of the MD Burgers vector parallel to the interface, $b_{\text{edge, } \parallel} = b \cos \lambda$, is equal to the misfit strain ε_m , i.e.,

$$\varrho_{\text{MD, relaxed}} b_{\text{edge, } \parallel} = \varepsilon_m. \quad (2)$$

For films of finite thickness that are grown on semi-infinite substrates, the equilibrium linear MD density $\varrho_{\text{MD, equil}}$ may be readily shown to scale in the following manner [4]:

$$\varrho_{\text{MD, equil}} = \varrho_{\text{MD, relaxed}} \left[1 - \frac{h_c}{h} \right]. \quad (3)$$

In the heteroepitaxial growth of semiconductors with large lattice mismatches, e.g., $\epsilon_m \gtrsim 2\%$, the critical thicknesses are less than 20 Å and dislocation generation is ubiquitous for layer thicknesses much in excess of h_c .

For layer-by-layer growth, the prevailing assumption is that dislocation half-loops nucleate at steps or impurities on the growing free surface [5, 6], and the loops expand to form two threading segments, largely of screw character, with antiparallel Burgers vectors, and a misfit segment at the film/substrate interface. Thus, the initial TD density is twice the nuclei density. For threading dislocation segments in epitaxial layers, we adopt the convention that the dislocation line direction is in the *same* sense as the film/substrate surface normal. This convention is used because in large mismatch heteroepitaxy it is practically impossible to identify matching pairs of TDs from the same nucleation event — that is, isolated loops are rarely, if ever, discernible. Dislocations with the same line sense but opposite (antiparallel) Burgers vectors are physical opposites and will annihilate upon contact. Further we treat the case in which the film thickness greatly exceeds the physically realized thickness in which MDs are generated, i.e., $h \gg h_k > h_c$. For buffer layers, we assume complete misfit relaxation in the film and only consider the possible reactions between the TDs. We note here that for $h > h_c$, the MDs are *equilibrium* interfacial defects with an equilibrium population given approximately by (3). On the contrary, the *TDs in all cases raise the free energy of the film* — the equilibrium density of these defects is zero.

2.2 Experiments on threading dislocations

In typical large mismatch semiconductor heteroepitaxy, the TD density is very high near the film/substrate interface and decreases with increasing film thickness. In recent years there have been several efforts to quantify the thickness dependence of the TD density for lattice mismatched growth. Sheldon et al. [7] reported on the thickness dependence of the TD density for the systems InAs/GaAs, GaAs/Ge/Si, GaAs/InP, and InAs/InP. These systems represented a range of lattice and thermal expansion mismatches between the film and the substrate. It was found that the TD density was proportional to the inverse of the film thickness for TD densities in the order of $\approx 10^8$ to 10^9 cm^{-2} . Further, the thickness dependence of the densities was found to fall on the same curve, independent of specific epilayer/substrate combination, as shown in Fig. 1a. In a similar study, Tachikawa and Yamaguchi [8] also observed the $1/h$ (where h is the film thickness) behavior for the TD density in thick films of GaAs on Si. However, at lower dislocation densities, a weaker decay was observed, as shown in Fig. 1b. Further, in the study of strained layer superlattices, TD densities have commonly been observed to saturate for larger film thickness [9 to 11]. Other data on experimental observations of the behavior of TDs are summarized in a recent review by Beanland et al. [1] where it was stressed that until now there has yet to be any reasonable model to explain the $1/h$ dependence of TD density in buffer layers.

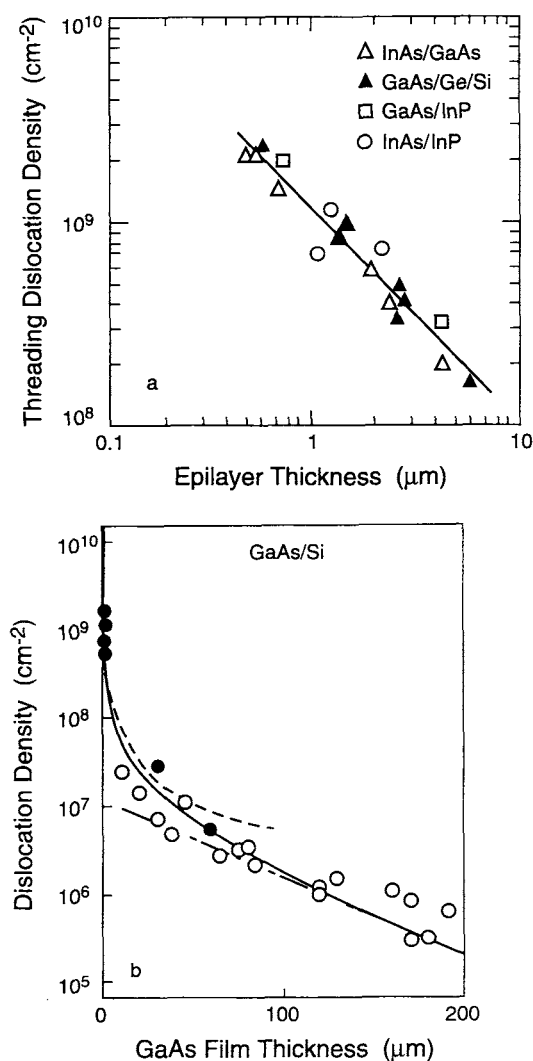


Fig. 1. Experimental data, reported in the literature, showing the scaling of the threading dislocation density with increasing film thickness. a) Results of a study showing the universal $1/h$ decay of the TD density for high dislocation densities for a range of systems (after Sheldon et al. [7]). b) Results of a study showing both the $1/h$ decay of the TD density for high dislocation densities and either saturation or exponential decay behavior of the TD density of thick films (after Tachikawa and Yamaguchi [8]).

3. Physical Basis for Threading Dislocation Density Reduction

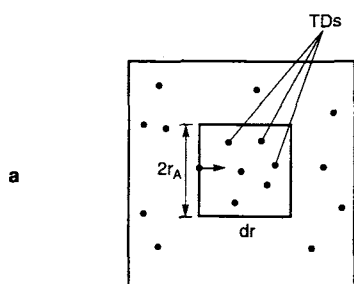
As we have mentioned above, TDs are non-equilibrium defects that always raise the internal energy of the film/substrate system. Thus, there is a natural driving force to reduce the internal energy and TD density, concomitantly. This reduction may, however, be achieved only as a result of kinetic processes, mainly by reactions between pairs of TDs. For reducing the total TD density, fusion and annihilation reactions are important. When two TDs fuse, they produce a single resulting TD; annihilation is only possible for TDs with opposite sign. The criteria for these reactions will be considered below. Here we only mention that both of these reactions can take place when the distance between interacting dislocations

becomes smaller than the characteristic cross-section of a specific reaction: annihilation radius r_A for annihilation reactions (the concept of the annihilation radius in the modeling of TD reduction was initially proposed by Martisov and Romanov [12]); fusion radius r_F for fusion reactions. After TDs have fallen within the interaction distance, they glide or climb together under the action of internal forces. There must be an initial relative motion for TDs to come within an interaction distance. During this motion, different barriers must be overcome. In addition to annihilation and fusion, one can consider scattering reactions among moving TDs. As the result of such a reaction, one or each of reacting TDs can change its direction of motion. We can also characterize the interaction length for scattering reactions by a scattering radius r_S . Both processes, motion and reaction, can be assisted by external and internal factors such as temperature, film growth geometry, internal and externally imposed stress, and point defects.

Usually we suppose that the reaction process between TDs requires less time than the "motion" process. This is because in order to initiate and continue TD motion high internal barriers (for example, high Peierls stresses for covalent semiconductors) must be overcome, as TDs come within an interaction distance, their motion is accelerated and becomes faster because the interaction forces are inversely proportional to the separation distance (as it follows from the consideration of the reactions between two straight parallel dislocations). Therefore, we may conclude that all approaches to TD density reduction rely upon enhancing TD motion such that TDs will fall within the interaction radius of one another. This is a necessary condition for all TD reduction processes. Using the concept of motion as an underlying principle, we will develop simple arguments for the general description of TD evolution in thin films.

First, to derive the governing equation for TD reduction, we consider only annihilation reactions. Assuming that the points of TD intersections with the film surface may experience relative motion (e.g., with increasing film thickness), each TD will sweep (see Fig. 2a) an interaction area $dS = 2r_A dr$, where dr is the differential value of the relative TD motion r . Each TD will encounter $dN = \rho \delta S$ other TDs where ρ is the density of TDs. Therefore, the change of TD density due to annihilation reactions will be

$$d\rho = -\rho dN = -2r_A \rho^2 dr. \quad (4)$$

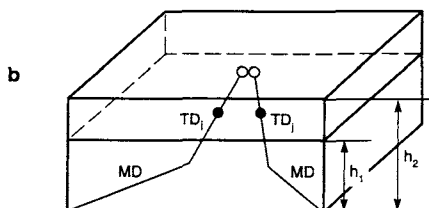


The relative motion r is a function of several parameters including time t , temperature T , film thickness h , stress tensor $\hat{\sigma}$, and other parameters, i.e.,

$$r = r(t, T, h, \hat{\sigma}, \dots) \quad (5)$$

and therefore

$$dr = \frac{\partial r}{\partial t} dt + \frac{\partial r}{\partial T} dT + \frac{\partial r}{\partial h} dh + \frac{\partial r}{\partial \hat{\sigma}} \bullet \bullet d\hat{\sigma} + \dots; \quad (6)$$



moreover there also can be internal relations between parameters that characterize the motion, and as we have mentioned previously, r_A can be a function of these parameters,

$$r_A = r_A(t, T, h, \hat{\sigma}, \dots). \quad (7)$$

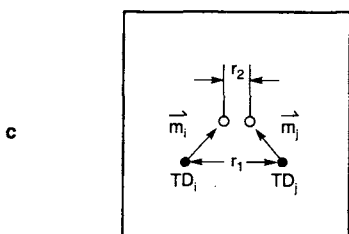


Fig. 2. Threading dislocation motion in growing films: a) The interaction area swept by a moving TD in plan view. Relative motion of inclined TDs as a result of film growth. b) Perspective view. c) Plan view. In b) and c) the positions of two TDs are shown for successive film thickness; $\mathbf{m}_i$ and $\mathbf{m}_j$ are unit vectors in the directions of the motion of TDs i and j along the film surface

Therefore, to find the dependence of TD density on external and internal parameters, one has to know the functional form of r and r_A (5) and (7). In the simplest cases, we can consider model functions for r and r_A . If $r = r(h)$, then we can arrive at the problem of TD reduction in strain-free buffer layers. Here we assume that changing film thickness, as a result of growth, is the only reason for TD motion. The effective motion of TDs is a consequence of the fact that each TD assumes a minimum energy line orientation (see below) which is constant during film growth. With increasing film thickness, the separation distance between the TDs will change, as shown in Fig. 2b and c, and at some film thickness, a minimum separation distance will be achieved. If the approach distance between two TDs with opposite Burgers vectors reaches a value of the annihilation radius r_A , TDs begin to glide together because of the attractive interaction and finally annihilate. If we assume that r_A is constant, then (4) may be written in the following form:

$$d\varrho = -K\varrho^2 dh, \quad (8)$$

where $K = 2r_A(\partial r/\partial h)$, and the partial derivative $\partial r/\partial h$ takes into account the geometry of TDs in the growing film. When K is not a function of h , (8) may be easily solved to provide the following dependence of TD density on film thickness:

$$\varrho = \frac{1/K}{h + \hat{h}}, \quad (9)$$

where $\hat{h} \equiv 1/(K\varrho_0) - h_0$, ϱ_0 is the TD density at the starting thickness h_0 , and h_0 usually can be taken as the thickness for which the average spacing between TDs is larger than the annihilation radius r_A . When $h \gg \hat{h}$, the TD density is inversely proportional to the film thickness, i.e.,

$$\varrho = \frac{1}{Kh}. \quad (10)$$

This simple approach thus predicts the $1/h$ scaling behavior. If we set K equal to twice the annihilation radius $2r_A$ ($\partial r/\partial h = 1$), we may readily solve for $\hat{h}$. For instance, if the initial threading dislocation density is 10^{10} cm^{-2} , $h_0 = 0$ (for simplicity), and the annihilation radius is $500 \text{ \AA}$, then $\hat{h}$ has a value of $1000 \text{ \AA}$. If we assume $h \gg \hat{h}$, (9) would be valid for thicknesses of the order of $1 \mu\text{m}$ and larger — this is in close agreement with the initial thicknesses for which TD densities are commonly reported. We note that the data of Sheldon et al. [7] shown in Fig. 1a correspond to an r_A value of $\approx 500 \text{ \AA}$ and the data of Tachikawa and Yamaguchi [8] shown in Fig. 1b correspond to an r_A value of $\approx 1000 \text{ \AA}$.

In close analogy to the simplified model developed above, Parts I and II of the present paper provide a detailed treatment of TD reduction in homogeneous buffer layers. In particular, the approach will not only include annihilation reactions but will also incorporate fusion and scattering reactions, and crystallographic details of the reactions between different families of TDs. The value of the rate constant K will be generalized. Finally, numerical solutions for TD density reduction will be found and analyzed.

Other methods of reducing TD densities (e.g., thermal annealing cycles, impurity doping, strained layer superlattices, and compositionally graded layers) can also be understood in the framework of relative TD motion. For these more involved approaches, the function for relative dislocation motion has to be determined in each particular case. Solution of these problems is the subject of our future work.

4. General Treatment of Inclined Threading Dislocations

4.1 Isolated threading dislocation

We begin by determining the orientation of an isolated TD in a film and then we derive the general geometry of interaction between pairs of TDs. First, consider a straight TD connected to a MD, as shown in Fig. 3. The Burgers vector $\mathbf{b}$ of this angular dislocation lies in its glide plane with normal $\mathbf{n}_g$, and thus, the TD is glissile. The free surface of the film has a normal $\mathbf{n}_f$ and the tangent vector of the TD is $\mathbf{l}$. Working under the assumption that the TD maintains a glissile orientation, the goal of this section is to determine the orientation of the TD line (unit vector $\mathbf{l}$). If $\mathbf{l}$ is known, then the angle ψ between the TD line and the surface normal may be found as

$$\psi = \cos^{-1} (\mathbf{l} \cdot \mathbf{n}_f). \quad (11)$$

If the position of the MD at the interface is fixed and we restrict the TD to be a straight line, there is an orientation for the TD that minimizes the energy of the TD-MD configuration. This minimum corresponds to the optimal balance between the screw component of a TD and its length (when the film thickness h is fixed). In a real situation, the energy of the TD-MD configuration has to be calculated by taking into account surface effects, the shape of the dislocation line, and differences in elastic properties between the film and the substrate. To find the simplified expression for the dislocation energy, we will work in an approximation of dislocation line tension [13] and neglect the interaction of the TD with the free surface and the interface. Taking the

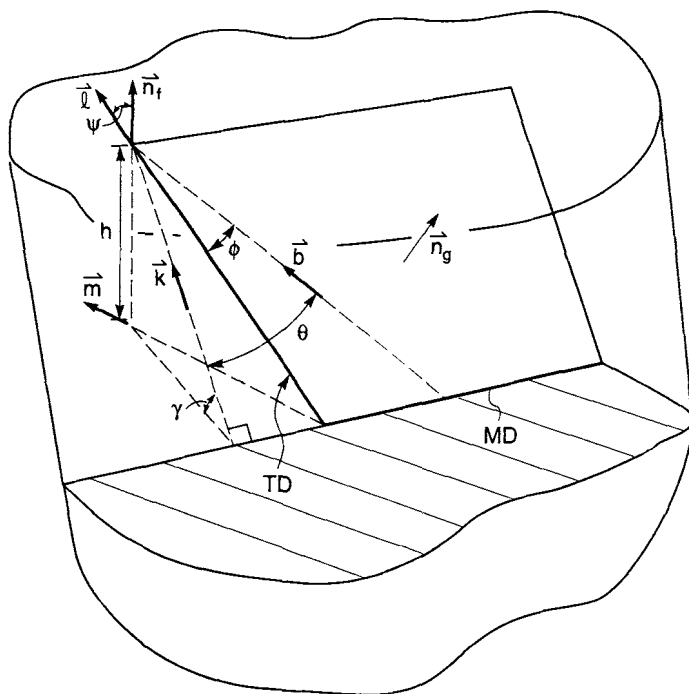


Fig. 3. Geometry of isolated TD-MD in the film/substrate system

angle ϕ between the TD line and its Burgers vector as the controlling parameter for the minimization of the dislocation energy, we can write the expression for this energy in the form

$$E(h, \phi) = \frac{\mu b^2}{4\pi} \frac{h}{\sin \gamma \cos(\theta - \phi)} \left(\cos^2 \phi + \frac{\sin^2 \phi}{1 - \nu} \right) \ln \left(\frac{\alpha R}{|b|} \right), \quad (12)$$

where μ is the shear modulus, ν is Poisson's ratio of the film, R is the screening length for the energy calculation, and the parameter α takes into account the contribution of the dislocation core (R depends weakly on h and ϕ but we neglect these dependencies because R is contained within the argument of the weakly varying logarithm function). The angles γ and θ can be found by considering the geometry of the shortest possible TD line in the slip plane (parallel to $\mathbf{k}$); γ is the angle between $\mathbf{k}$ and the projection of $\mathbf{k}$ to the film/substrate interface,

$$\gamma = \cos^{-1}(\mathbf{n}_g \cdot \mathbf{n}_f), \quad (13)$$

and θ is the angle between $\mathbf{b}$ and $\mathbf{k}$,

$$\theta = \cos^{-1} \left(\frac{\mathbf{b} \cdot \mathbf{n}_f}{|b| \sin \gamma} \right). \quad (14)$$

After the angle ϕ is found from the minimization of (12), we can then derive the relation for the unit vector $\mathbf{l}$ along the TD line,

$$\mathbf{l} = \frac{\sin(\theta - \phi)}{\sin \theta} \frac{\mathbf{b}}{|b|} + \frac{\sin \phi}{\sin \theta} \mathbf{k}, \quad (15)$$

where $\mathbf{k}$ is also given as

$$\mathbf{k} = \frac{\mathbf{n}_g \times (\mathbf{n}_f \times \mathbf{n}_g)}{\sin \gamma}. \quad (16)$$

During continuing film growth, we propose that the geometry of the TD-MD system remains self-similar. This means that the TD remains in the position of minimum energy with constant angle ϕ and therefore constant line direction $\mathbf{l}$. The point of intersection of the inclined TD with the free surface will, however, move along the free surface with increasing film thickness, as shown schematically in Fig. 2. Thus, even in the absence of glide, there is lateral motion (in the laboratory reference frame) of the inclined TD with increasing film thickness. The direction of this motion $\mathbf{m}$ in the surface plane is given as

$$\mathbf{m} = \frac{\mathbf{l} - (\mathbf{l} \cdot \mathbf{n}_f) \mathbf{n}_f}{|\mathbf{l} - (\mathbf{l} \cdot \mathbf{n}_f) \mathbf{n}_f|}. \quad (17)$$

4.2 Relative motion and reactions of threading dislocations

Consider now two TDs with Burgers vectors $\mathbf{b}_i$ and $\mathbf{b}_j$ and line directions $\mathbf{l}_i$ and $\mathbf{l}_j$, as shown in Fig. 2b. At film thickness h_1 , TD_i and TD_j are separated by a distance r_1 . At film thickness h_2 , the two TDs are separated by a distance r_2 , as shown in Fig. 2c. If the TDs come within a distance such that the interaction forces are sufficient to initiate additional motion of dislocations, then they can start to react to produce new dislocations or change their trajectories of motion. The minimum distance to initiate disloca-

tion motion is referred to as the interaction radius r_I . Different types of interactions are possible between TDs and include: (i) annihilation, (ii) fusion reactions, and (iii) scattering reactions. The possibility of reactions is primarily governed by Frank's rule (the b^2 criterion) [13]. A reaction between TD_i and TD_j to produce a new TD_k with Burgers vector $\mathbf{b}_k = \mathbf{b}_i + \mathbf{b}_j$, should fulfil the condition

$$b_k^2 \leq b_i^2 + b_j^2. \quad (18)$$

In the case that $\mathbf{b}_k = 0$, we have an *annihilation* reaction and the corresponding interaction distance is referred to as the annihilation radius r_A . For the case $\mathbf{b}_k \neq 0$ and $b_k^2 < b_i^2 + b_j^2$, we have a *fusion* reaction and the corresponding interaction distance is referred to as the fusion radius r_F . Fusion reactions lead to an overall TD density reduction. In the case that $b_k^2 > b_i^2 + b_j^2$, there will be no annihilation or fusion reactions of TDs, however, the local scattering (change of TD trajectories of their motion) can take place. Scattering reactions will have a characteristic interaction distance that will be referred to as the scattering radius r_S . Finally, for the case $b_k^2 = b_i^2 + b_j^2$, the principles of minimization of dislocation length contribution become important. Here, the outcome of the possible reaction will be dictated by the dislocation core energy dependence on the value of the Burgers vector together with minimization of a dislocation length for a given film thickness.

To find the value of the interaction radii, r_A , r_F , and r_S , we must solve the complicated problem of the interaction of two angular TD-MDs near a free surface. Factors such as temperature, Peierls barrier, internal and externally imposed stress, presence of point defects must all be considered. We will begin to treat these problems in our future work.

Here we explore the approach dealing with TD densities and making an analogy to simple chemical reaction kinetics. Again, consider TDs of the i -th and j -th types with corresponding densities ϱ_i and ϱ_j . We suppose that due to the effective motion of inclined TDs the reactions occur with uniform probability at any point on the surface with prescribed reaction velocity V_{ij} . Then for diminishing defect densities ϱ_i or ϱ_j as a result of the direct reaction of RDs of the i -th and j -th types we can write

$$\frac{d\varrho_{i(j)}}{dt} = -V_{ij}\varrho_i\varrho_j. \quad (19)$$

The reaction velocity can be expressed via relative dislocation motion and interaction cross-section r_I in the following form:

$$V_{ij} = 2r_I |\mathbf{V}_i - \mathbf{V}_j|, \quad I = A, F, \text{ or } S, \quad (20)$$

where $\mathbf{V}_i$ and $\mathbf{V}_j$ are the velocities of motion of the TD intersections with the free surface as a result of film growth. The velocity of a TD can be written as

$$\mathbf{V}_j = \dot{h} \tan(\psi_j) \mathbf{m}_j, \quad (21)$$

where $\dot{h} = dh/dt$ is the film growth rate. After that, the expression for the decrease of density of dislocations participating in the reaction (19) can be rewritten in the form directly connecting densities and film thickness,

$$\frac{d\varrho_{i(j)}}{dh} = -K_{ij}\varrho_i\varrho_j, \quad (22)$$

where the “kinetic” coefficient K_{ij} is given as

$$K_{ij} = 2r_l |\tan \psi_i \mathbf{m}_i - \tan \psi_j \mathbf{m}_j| \quad (23)$$

which can also be written as

$$K_{ij} = 2r_l \left| \frac{\sqrt{1 - (\mathbf{l}_i \cdot \mathbf{n}_f)^2}}{|\mathbf{l}_i \cdot \mathbf{n}_f|} \frac{[\mathbf{l}_i - (\mathbf{l}_i \cdot \mathbf{n}_f) \mathbf{n}_f]}{|\mathbf{l}_i - (\mathbf{l}_i \cdot \mathbf{n}_f) \mathbf{n}_f|} - \frac{\sqrt{1 - (\mathbf{l}_j \cdot \mathbf{n}_f)^2}}{|\mathbf{l}_j \cdot \mathbf{n}_f|} \frac{[\mathbf{l}_j - (\mathbf{l}_j \cdot \mathbf{n}_f) \mathbf{n}_f]}{|\mathbf{l}_j - (\mathbf{l}_j \cdot \mathbf{n}_f) \mathbf{n}_f|} \right|. \quad (24)$$

Analyzing the expression for K_{ij} , we conclude that it reflects all essential features of the TD geometry. First, for perpendicularly oriented TDs, $\mathbf{l}_i = \mathbf{l}_j = \mathbf{n}_f$, there will be no motion and correspondingly no interaction of the TDs; therefore, $K_{ij} = 0$ in this case. Second, for $\mathbf{l}_i = \mathbf{l}_j \neq \mathbf{n}_f$, there will be no relative dislocation motion and again $K_{ij} = 0$.

The reactions of the type given in (19) will also contribute to the production of TDs: in the case of fusion reactions, TDs of a new type ϱ_k will appear; in the case of scattering reactions, TDs of a new type may be generated by cross slip of existing TDs (conservation of Burgers vector, change of slip plane). For the case of scattering reactions, the total number of interacting dislocations does not change. In the case of annihilation, no new TDs are produced as a result of the reactions. The TD *production* terms can be taken into account with the help of an additional set of coefficients β_{ij}^k

$$\frac{d\varrho_k}{dh} = \beta_{ij}^k K_{ij} \varrho_i \varrho_j. \quad (25)$$

Based on this discussion, we can conclude that for annihilation reactions $\beta_{ij}^k = 0$, for fusion reactions $\beta_{ij}^k = 1$ ($k \neq i, k \neq j$) and for scattering reactions $\beta_{ij}^k + \beta_{ij}^m + \beta_{ij}^i + \beta_{ij}^j = 2$, where k and m correspond to dislocations that can appear as a result of scattering of the i -th and j -th dislocations.

5. Dislocation Geometry and Reactions for (001) F.C.C. Film Growth

The most common growth orientation for semiconductor heteroepitaxy is (001). Thus, in this paper, we restrict our study to cube-on-cube epitaxy of f.c.c. materials. For f.c.c. semiconductors, such as Si, Ge, or GaAs, the most common slip system is $a/2 \langle 110 \rangle \{111\}$. The Burgers vectors for this system are along the face diagonals of the cubic cell and represent the shortest possible primitive lattice translation vectors. The possible set of Burgers vectors for the f.c.c. system are parallel to the edges of a half octahedron, as shown in Fig. 4a. The half-octahedron is oriented such that the square base is parallel to the (001) plane and the inclined faces are parallel to either (111), ($\bar{1}11$), ($1\bar{1}1$), or ($\bar{1}\bar{1}1$).

As was mentioned in Section 2.1, we consider the possibility that MDs and TDs are generated by surface-related processes for layer growth and possibly by lateral injection mechanisms in island growth. For layer growth, misfit strains in coherent or partially relaxed films may be relieved by surface nucleation of dislocation half-loops. Assuming homogeneous biaxial tension, the half-loops will form on inclined slip planes with Burgers vectors that are inclined with respect to the film substrate interface. For the (001) growth of f.c.c. semiconductors, this plane corresponds to one of the four inclined faces of the half-octahedron shown in Fig. 4a and the possible Burgers vector of the disloca-

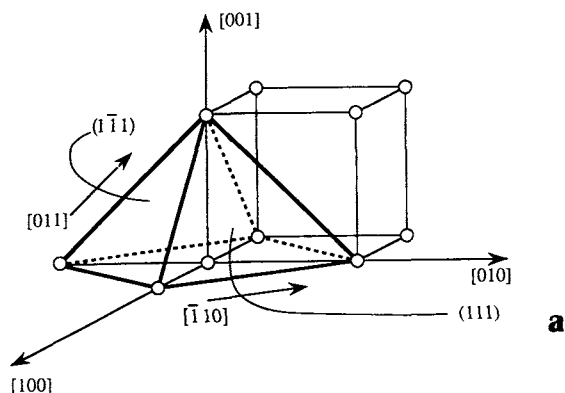
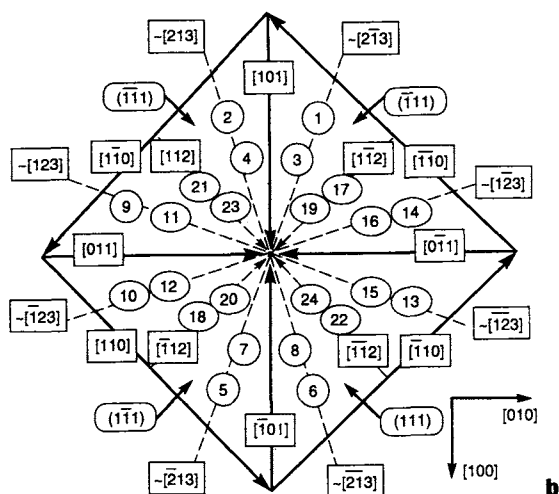


Fig. 4. a) $\langle 001 \rangle$ deformation half-octahedron. b) Projection down $[001]$ of the deformation half-octahedron



tions will be one of the following: $\pm a/2 [101]$, $\pm a/2 [011]$, $\pm a/2 [\bar{1}01]$, $\pm a/2 [0\bar{1}1]$. For dislocation half-loop nucleation at the film surface, the Burgers vectors of the half-loop, and eventually the pair of TDs and the MD, will be parallel to one of the inclined half-octahedron edges (note again, however, that we use the uncommon convention that the line directions of the TD segments are in the same sense as the surface normal, and thus the two TD segments for a half-loop will have opposite sense Burgers vectors). This gives the set of possible Burgers vectors for surface nucleation as: $\pm a/2 [101]$, $\pm a/2 [011]$, $\pm a/2 [\bar{1}01]$, $\pm a/2 [0\bar{1}1]$. For island growth, there is the additional possibility that the MDs are generated by a lateral injection mechanism at the island periphery, thus the initial set of MDs may have their Burgers vectors lying in the film/substrate interface. This set of Burgers vectors will be parallel to one of the edges of the square base of the half-octahedron and will be from the set $\pm a/2 [110]$, $\pm a/2 [\bar{1}\bar{1}0]$. TDs may be generated as a result of island coalescence with the same possible Burgers vectors as those of the MDs. Within the context of island growth, we do not exclude the possibility of nucleating dislocations at the free surface of an island.

For f.c.c. systems, the Burgers vectors can lie on one of two slip planes. Although there are 12 unique Burgers vectors, there are 24 Burgers vectors/slip plane combina-

tions. Thus, in considering the overall reactions between TDs, a 24×24 matrix can be constructed to investigate all possible TD-TD interactions. Before considering the possible reactions between TDs, it is first important to analyse the orientational dependence of the energy of an inclined TD.

Dislocations must terminate at other dislocations, high-angle grain boundaries, or free surfaces. Specifically, an isolated dislocation line cannot terminate within a crystal. Assuming that a TD is anchored at, or near, the film/substrate interface, it must either thread to the free surface of a film, fuse with another TD to form a third TD segment, or form a loop that closes back down on the interface. For the case in which the TD threads to the free surface, the energy of the TD is a balance between minimizing line length while concurrently maximizing the screw character. For (001) film growth, all $\{111\}$ slip planes have the same inclination with respect to $\mathbf{n}_f$. Thus we need to consider only the orientation for minimum energy of TDs with Burgers vectors that are parallel to the film/substrate interface $\mathbf{b}_p$ (e.g., $a/2 [\bar{1}10]$) or those which are inclined $\mathbf{b}_i$ (e.g., $a/2 [\bar{1}01]$). For these two types of dislocations, the angles γ and θ in the expression for TD energy (see (12)) will be correspondingly $\gamma_p = \gamma_i = \sin^{-1}(\sqrt{2}/\sqrt{3})$, $\theta_p = \pi/2$, $\theta_i = \pi/6$. In Fig. 5 we plot the dependence of TD energy on orientation for TDs with Burgers vectors that are either parallel or inclined with respect to the film/substrate interface (a Poissons ratio value of 0.3 was used here). For TDs with their Burgers vector parallel to the film/substrate interface, the minimum energy orientation is parallel to $\mathbf{k}$, the direction of shortest line length. For the $\{111\}$ family of slip planes, this orientation corresponds to a TD line direction parallel to $\langle 112 \rangle$. For TDs with inclined Burgers vectors, the minimum energy orientation is $\approx 15^\circ$ away from $\mathbf{b}$ in the sense that reduces line length and we will approximate this direction, for (001) films, as $\langle 123 \rangle$ where the third Miller index is always 3 and positive. On this basis, the motion of the

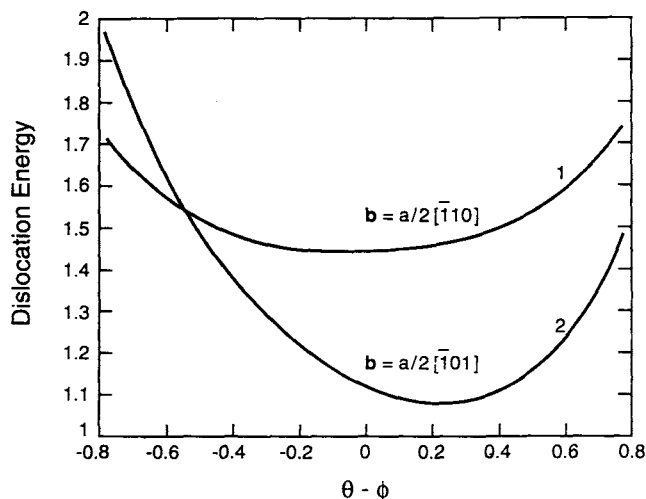


Fig. 5. Dependence of TD energy in (001) films on the deviation of the TD orientation from the shortest line length orientation. The TDs in this case are in the $\{111\}$ plane. Curve 1 corresponds to a TD with a Burgers parallel to film/substrate interface $\mathbf{b}_p = a/2 [\bar{1}10]$. Curve 2 corresponds to a TD with a Burgers inclined to film/substrate interface $\mathbf{b}_i = a/2 [\bar{1}01]$. The energy is in units of $(\mu b^2 h \sqrt{3}/4\pi \sqrt{2}) \ln(\alpha R/|b|)$

Table 1

Reactions between threading dislocations in (001) epitaxial f.c.c. semiconductor films. The TDs have $a/2\langle 101 \rangle$ Burgers vectors. TDs 1 through 16 correspond to those generated by surface half-loop nucleation and have approximate line directions $\parallel$ parallel to $\langle 123 \rangle$. TDs 17 through 24 correspond to those generated by island growth or by fusion reactions and have line directions $\parallel$ parallel to $\langle 112 \rangle$

#	$I_s \parallel$	b_i/b_j	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
#	$I_s \parallel$	b_i/b_j	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$	$a/2[101]$
1	$[2\bar{1}3]$	$a/2[101]$	U	S1	U	0	N	N	N	S2	S2	21	S2	S2	17	S2	14	S2	9							
2	$[213]$	$a/2[101]$	S1	U	0	U																				
3	$[2\bar{1}3]$	$a/2[101]$	U	0	U	S1	N	N	N	23	S2	S2	19	S2	16	S2	11	S2								
4	$[213]$	$a/2[101]$	0	U	S1	U																				
5	$[2\bar{1}3]$	$a/2[101]$	N		N	U	S1	U	0	S2	20	S2	S2	24	10	S2	13	S2								
6	$[213]$	$a/2[101]$	N		N	S1	U	0	U																	
7	$[2\bar{1}3]$	$a/2[101]$	N		N	U	0	U	S1	18	S2	S2	22	S2	12	S2	15									
8	$[213]$	$a/2[101]$	N		N	0	U	S1	U																	
9	$[123]$	$a/2[011]$	S2	23	S2	S2	18			U	S1	U	0	N	N	S2	5	S2	2	S2						
10	$[123]$	$a/2[011]$	S2	21	S2	20	S2	20	S1	U	0	U	S1	N	N	7	S2	4								
11	$[123]$	$a/2[011]$	21	S2	20	S2	20	U	0	U	S1	U														
12	$[123]$	$a/2[011]$	21	S2	20	S2	20	U	0	U	S1	U														
13	$[123]$	$a/2[011]$	S2	19	S2	22	S2	22	N	N	U	S1	U	0	1	S2	6									
14	$[123]$	$a/2[011]$	S2	17	S2	24	S2	24	N	N	U	0	U	S1	U	3	S2	8	S2							
15	$[123]$	$a/2[011]$	17	S2	16	10	S2	10	S2	12	S2	7	1	S2	3	S2	N									
16	$[123]$	$a/2[011]$	17	S2	16	10	S2	10	S2	12	S2	7	1	S2	3	S2	N									
17	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
18	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
19	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
20	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
21	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
22	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
23	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U
24	$[112]$	$a/2[110]$	S2	14	S2	13	S2	13	S2	2	S2	4	6	S2	N	N	U	S1	U	0	U	S1	U	U	U	U

The following notations are used for the table entries: U: parallel dislocation lines $\parallel$ — geometrically unlikely for annihilation, fusion, or scattering; S1: repulsion (from b^2 criterion) — scattering of dislocations with the same Burgers vector; S2: repulsion (from b^2 criterion) — scattering of dislocations with different Burgers vector; N: no reaction (from b^2 criterion), however, possible fusion or scattering; 0: annihilation reaction; #: fusion reaction, the number corresponds to the resulting dislocation

TDs on the growing film surface is determined by (17). The minimum energy orientation for all 24 possible TDs for (001) f.c.c. films is shown in Fig. 4b. The labeling scheme used for the TDs is given in Table 1.

The possible reactions between TDs are based on both their geometric likelihood of interaction and whether the possible reactions are energetically favorable. As described earlier, the b^2 criterion is used to determine whether or not reactions are favorable. All annihilation reactions lead to energy release and thus are favorable. For favorable fusion reactions, the resulting TD may have a Burgers vector that can lie on several different slip planes. We argue that the slip plane the TD chooses is such that the line direction of the resulting TD most closely maintains force balance at the node of the three TD junctions. Finally, repulsive reactions are determined by both unfavorable energies and additional Burgers vectors that have an acute angle. Repulsive interactions between TDs may lead to a change in slip plane for a given TD, a process that we refer to as scattering. Using these criteria, the reactions between pairs of TDs can be developed and are shown in Table 1. In this table, the following notation is used: U corresponds to parallel dislocation lines l with no geometrical likelihood for interaction; S1 and S2 correspond to repulsive interactions (from b^2 criterion) and may lead to scattering; N corresponds to no reaction (from the b^2 criterion), however, there is a possibility for fusion or scattering; 0 corresponds to annihilation reactions; and finally the entries with a specific number correspond to the resulting TD from a fusion reaction.

6. Summary and Conclusions

This paper offers the geometric possibility for reactions between TDs as a result of film growth. The reactions become possible if pairs of TDs come within a critical distance: r_A for annihilation reactions, r_F for fusion reactions, and r_S for scattering reactions. The effective motion of an inclined individual TD in a stress-free homogeneous layer has essentially a purely geometrical origin. In cases where the inclined TD maintains a constant line direction, the point of intersection of the TD with the film free surface will move laterally on the film surface with increasing film thickness. Since the line directions for different TDs may be different, this results in mutual dislocation motion in TD ensembles.

The simplified model based on the ability of TDs to move has been proposed to explain the experimentally observed $1/h$ dependence of TD density. In this Part I of the paper, the parameters describing dislocation motion have been found for arbitrarily oriented TDs. After that, these general results were applied to the case of (001) epitaxial growth of f.c.c. semiconductors together with considerations of the crystallography of possible reactions between TDs.

The results from Part I will be used in Part II for the derivation of a series of coupled differential equations that describe the details of TD density evolution in homogeneous buffer layers.

Acknowledgements This work was supported in part by the UC MICRO program in conjunction with Hughes Aircraft corporation, by the AFOSR through contract F49620-95-1-0394 (Dr. Gerald Witt contract monitor) and by the Max Planck Society. Additional support for GEB was provided by an Alexander-von-Humboldt Fellowship.

References

- [1] R. BEANLAND, D. J. DUNSTAN, and P. J. GOODHEW, *Adv. Phys.* **45**, 87 (1996).
- [2] J. S. SPECK, M. A. BREWER, G. E. BELTZ, A. E. ROMANOV, and W. POMPE, *J. appl. Phys.* **80**, 3808 (1996).
- [3] L. B. FREUND, *MRS Bull.* **17**, 52 (1992).
- [4] J. Y. TSAO, *Materials Fundamentals of Molecular Beam Epitaxy*, Academic Press, New York 1993.
- [5] T. J. GOSLING and J. R. WILLIS, *J. Mech. Phys. Solids* **42**, 1199 (1994).
- [6] G. E. BELTZ and L. B. FREUND, *phys. stat. sol. (b)* **180**, 303 (1993).
- [7] P. SHELDON, K. M. JONES, M. M. AL-JASSIM, and B. G. YACOBI, *J. appl. Phys.* **63**, 5609 (1988).
- [8] M. TACHIKAWA and M. YAMAGUCHI, *Appl. Phys. Letters* **56**, 484 (1990).
- [9] H. OKAMOTO, Y. WATANABE, Y. KADOTA, and Y. OHMACHI, *Japan. J. appl. Phys.* **26**, L1950 (1987).
- [10] N. HAYAFUJI, S. OCHI, M. MIYASHITA, M. TSUGAMI, T. MUROTANI, and A. KAWAGISHI, *J. Crystal Growth* **93**, 494 (1988).
- [11] N. HAYAFUJI, M. MIYASHITA, T. MISHIMURA, K. KADOIWA, H. KUMABE, and T. MUROTANI, *Japan. J. appl. Phys.* **29**, 2371 (1990).
- [12] M. Y. MARTISOV and A. E. ROMANOV, *Soviet Phys. — Solid State* **32**, 1101 (1990).
- [13] J. P. HIRTH and J. LOTHE, *Theory of Dislocations*, 2nd ed., Wiley, New York 1982.