Strain relaxation models

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Contents

1 Misfit strain accomodation

The lattice mismatch for the semiconductor layer with lattice constant a is measured by the misfit parameter f_m

$$f_m = \frac{a - a_s}{a_s}$$

where a_s is the lattice constant of the substrate. The misfit parameter for the Ge_xSi_{1-x}/Si heterostructure could be written, using Vegard rule $a(x) = xa_{Ge} + (1 - x)a_{Si}$, as $f_m = 0.418x$.

If the thickness h of the layer is small, the misfit between the two semiconductors is accommodated by a strain of the layer that is known as the 'misfit strain'. The in-plain $(x - y)$ components of the strain tensor are

$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{\parallel} = f_m$$

while the normal one

$$\varepsilon_{zz} = \varepsilon_{\perp} = -2\frac{C_{13}}{C_{33}}\varepsilon_{\parallel} = -\frac{2\nu}{1 - \nu}\varepsilon_{\parallel}$$

where C_{ij} are the components of the elastic stiffness tensor in Voigt notation [1] and ν is the Poisson ratio that can differ significantly from its bulk value for very thin films [2]. Subscript $\parallel$ will be omitted below.

The general definition of the elastic energy is

$$E^{el} = \frac{1}{2}\mathcal{E} \cdot \mathcal{C} \cdot \mathcal{E}.$$

The elastic energy E per unit area stored in the layer due to the homogeneous strain is [3]

$$E^{el} = Bhf_m^2$$

where the constant B is defined as

$$B = 2\mu\frac{1 + \nu}{1 - \nu}$$

and μ is the elastic shear modulus. B is not the bulk modulus: it allows for the vertical relaxation of the layer which accompanies the constraint in the plane, and incorporates the factor of $1/2$ in relating elastic energy to the square of strain.

The strain energy E^{el} is proportional to h. As h increases and exceeds a certain critical thickness h_c, pseudomorphic growth of the uniform layer with flat free surface is no more possible and several phenomena are observed:

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- introduction of misfit dislocations

- modulation of the free surface profile

- composition modulations [4, 5, 6]

- microtwin formation [7, 8]

- interdiffusion between the layer and the substrate [9, 10]

The last mechanism usually occurs at temperatures higher than typical growth ones. The composition nonuniformities and microtwin formation are of primary interest for III-V ternary compounds when one of the constituents is In. Ref. [11] lists reasons to ignore concentration fluctuations in an analysis of SiGe morhology, the first one being a well-known fact that Si and Ge are miscible over the entire composition range. Thus models of the last three mechanisms are not discussed below.

Strain relaxation through misfit dislocations and through the surface modification are certainly the major routes for the strain accomodation in SiGe alloy. As a rule of thumb, the first one dominates for low while the second - for high lattice mismatch. However, these mechanisms, depending on the materials system, growth temperature and the value of the misfit strain could be cooperative as well as competitive [12, 13, 14]. On the one hand, there is a direct correlation between the surface cross-hatched morphology and the arrangement of the interfacial misfit dislocations [15]; surface undulations, in turn, could serve as nucleation sites. On the other hand, strain relief by one of this mechanism reduces the driving force for the other.

The strain, surface and interface energies of the SiGe/Si heterostructure with and without misfit dislocations have been recently computed for all three growth modes (Frank-van der Merve, Stranski-Krastanov and Volmer-Weber) as a function of the layer composition and thickness [16].

Introduction of misfit dislocations could be explained by an analysis of the energy of the system. For $h > h_c$ introduction of dislocations becomes energetically favourable providing a partial strain accommodation. They are introduced at the interface in the case of the constant layer composition and throughout the strained graded layer (uniformly when the linear grading is used and non-uniformly for the square-root or parabolic profile [17]).

Misfit dislocations could be produced by the motion of the threading dislocations from the substrate or generated in the strained layer via nucleation and/or multiplication. Three stages (regimes) of the strain relaxation

through introduction of misfit dislocations can be distinguished [18, 19]. The first one is characterised by a relatively slow strain relief provided mainly by the glide of the pre-existing threading dislocations. The relaxation rate in the second one is higher and depends on the multiplication processes and activization of new nucleation mechanisms. In the last stage a saturation of relaxation is observed caused by the strain hardening ('work-hardening') [20].

On the other hand, the elastic energy of a body with a flat surface *always diminishes* if the surface becomes wavy and thus counteracts the effect of increasing surface energy. Thus the strained flat surface could be unstable and development of surface undulations could relax strain. The wavelenth λ of the surface ripples is decrease with the layer strain [21]: $\lambda \propto \varepsilon^{-2}$. The strain is reduced locally at the peaks of the structure and is increased in the throughs.

An extreme stage of surface roughening is the formation of epitaxial islands that are a promising object for electronic devices [22]. This problem had gain a lot of attention recently (see, for example, reviews [23, 24, 25]). The reverse phenomenon - strain relaxation by pit formation in the compositionally graded SiGe thick films - also has been observed [26, 27]. Island coalescence could lead to the formation of the crystallographic tilt due to the asymmetric generation of 60° dislocation and asymmetric strain relief [28]. It is believed that in contrast to InGaAs strained layers that are characterized by an instability against the simultaneous perturbation of the surface profile and the composition, the onset of the surface roughening of strained the SiGe layers is primarily determined by nucleation of islands [29]. Surface roughening is certainly an evil, if the aim is to grow a planar layer.

2 Dislocation system in equilibrium

Two theories have been developed to calculate the equilibrium critical thickness h_c of the uniform epitaxial layer. The first theory originated in the work of Frank and Van der Merwe [30] and has been developed further by Van der Merwe and collaborators [31]. It is based on the principle of the energy minimization. The second one by Matthews and Blakeslee [32, 33] is known as the force balance theory. Being correctly formulated, these two theories are equivalent and give the identical critical thickness, as by definition of thermodynamic equilibrium they must. It has been shown that the expres-

sion for the critical thickness could be also used for graded layers if the misfit parameter is based on the average Ge concentration [34]. Subsequent development of critical thickness models has been aimed at the accurate modelling of the dislocation core energy [35], accounting for the surface effects [36] and anisotropy [37].

If the thickness of the layer is continuously increased, the energy minimization predicts that the number of misfit dislocations and the strain relaxation will also increase. The strain is never fully relaxed for any finite value of the thickness but approaches f_m (which corresponds to the complete relaxation of strain) as h tends to ∞. To calculate the number of dislocations as a function of h, a minimum of the total energy of the layer should be determined.

The possible orientations of the misfit dislocations are limited by the crystallography of the system. For the f.c.c. structures of SiGe alloys with the interface normal coinsiding with a cube edge dislocations form in two parallel arrays with members of one array being perpendicular to the members of the other. Let the spacing between two neighbouring dislocations in the arrays be p and

$$b_1 = -b\sin(\alpha)\sin(\beta),$$

where b is Burgers vector, α is the angle between the glide plane and the normal to the interface and β is the angle between the dislocation line and the Burgers vector [38, 39]. For 60° dislocations

$$\alpha = \arctan\frac{1}{\sqrt{2}}, \qquad \beta = \frac{\pi}{3}$$

while for 90° dislocations

$$\alpha = \frac{\pi}{2}, \qquad \beta = \frac{\pi}{2}$$

The in-plain component of the homogeneous strain in the layer in the presence of dislocations becomes

$$\varepsilon = f_m + \frac{b_1}{p}$$

and the energy

$$E = Bh\left(f_m + \frac{b_1}{p}\right)^2.$$

f_m and b_1/p always have opposite signs and the homogeneous energy is reduced by the misfit dislocations (misfit-energy-increasing dislocations studied

in ref. [40] are nonequilibrium ones). The energy of dislocations E^{d} is determined using linear elasticity (for example, [41, 42]). It also contributes to the total energy that for uniform distribution of dislocations is written as

$$E^{\mathrm{tot}} = Bh \left(f_m + \frac{b_1}{p} \right)^2 + \frac{2}{p} E^{\mathrm{d}}.$$

In the early works the following expression for the dislocation energy has been used

$$E^{\mathrm{d}}_{\infty} = Ab^2 \left((1 - \nu \cos^2 \beta) \left(\ln \frac{\varrho h}{b} + 1 \right) \right) \tag{1}$$

where $A = \mu/(4\pi(1-\nu))$ and parameter ϱ accounts for the non-elastic energy of the dislocation core. Note that the energy only weakly depends on the concrete value of ϱ for $h \gg b$.

A number of both explicit and implicit assumptions have been made in derivation of this relation and folowing from it equation for the critical thickness

$$h_c = \frac{b(1 - \nu \cos^2 \beta) \left(\ln \dfrac{\varrho h}{q} + 1 \right) + \dfrac{8\pi(1 - \nu^2)s\gamma}{Bb(1 - \nu)}}{8\pi(1 + \nu) \sin \beta \sin \alpha \left(f_m - \dfrac{2}{B} \dfrac{\sigma^{\widetilde{\mathrm{fault}}}}{b \cos(2\alpha) \sin \beta} \right)} \tag{2}$$

Often the step energy and the stacking fault energy in eq. (2) are omitted.

One of the simplifying assumption in the derivation of eqs. (1,2) is the neglection of the interaction between dislocations. Accounting for this effect leads to [66]

$$E^{\mathrm{d}} = A \left[a_0 + a_1 \ln \left(p \frac{1 - \exp(-g)}{2\pi q} \right) + a_2 \frac{g \exp(-g)}{1 - \exp(-g)} - a_3 \frac{g^2 \exp(-g)}{(1 - \exp(-g)^2} - a_2 \right]$$

where

$$a_0 = (b_1^2 + b_2^2) \left(\sin^2 \alpha - \frac{1 - 2\nu)}{4\pi(1 - \nu)} \right), a_1 = b_1^2 + b_2^2) + (1 - \nu)b_3^2,$$

$$a_2 = b_1^2 - b_2^2, a_3 = \frac{1}{2}(b_1^2 + b_2^2), g = 4\pi \frac{h}{p}, b_2 = b \cos \alpha \sin \beta, b_3 = -b \cos \beta.$$

Recently it has been claimed, however, that this expression overestimate the effect of dislocation interactions [43].

The relations displayed so far ignore the presence of the free surface. This drawback has been eliminated in ref. [44] using the image method. However, in this work, in turn, it has been assumed implicitly that the substrate has the infinite thickness. This restriction seems to be too severe nowadays due to the importance that have gained so called *compliant* substrates. The problems related to the use of such substrates ("strain partitioning", critical thickness reduction) have been analyzed recently in ref. [45].

The most rigorous analysis of the critical thickness is probably presented in ref. [46] where the finite thickness of both the substrate and the epitaxial layer as well as the difference in mechanical properties are taken into account.

In the capped layers relaxation occurs by the introduction of dislocation dipoles (the expression for the dipole energy could be found in ref. [66]). When the cap layer thickness is less than a certain thickness, a mixture of the single and paired misfit dislocations has been observed [47].

The regular periodic distribution having the lowest energy is rarely occurs in real systems: the dislocations frequently nucleate at regenerative heterogeneous sources (defects, impurities, ledges etc.), and hence form bunches. Presumably, these bunches are distributed in a random manner in the layer. For example, statistically significant measurements of ref. [48] reveal that distribution of spacings, being a broad unimodal one at the begining of the strain relaxation, could tend to a bimodal distribution as the misfit relief proceeds (the mean spacing decreases) while in [49] only significant narrowing of the unimodal distribution has been registered.

The energy of the non-periodic dislocation arrays has been considered in [50]. The total energy of a layer containing non-periodic arrays can be calculated by adding the homogeneous misfit strain energy and the interaction energy between the homogeneous misfit strain and the average strain caused by the dislocation arrays. In equilibrium the number of misfit dislocations in the layer is smaller if the distribution is non-periodic.

The primary use of the expression for the total energy of the layer containing dislocations, as was indicated, is to determine the critical thickness at which dislocations should appear. However, one can also get the concentration of dislocation $1/p_e$ that cause strain relaxation $|b_1/p_e|$ and thickness h_e for the equilibrium 'supercritical' layers ($h > h_c$) [38]. The values $|b_1/p_e|$ that provide energy minimum increase with h first rapidly and then slowly. For any given thickness, the concentration of dislocations $1/p_e$ is smaller if interactions of dislocations are not properly taken into account. The observed concentrations are always much smaller than the predicted values for

a periodic distribution. The discrepancy is partly due to the non-periodic distribution and partly due to the difficulty in nucleating the dislocations.

The effect of the finite size of the substrate or mesa on the dislocation density reduction [51] has been considered analytically in ref. [52] where the distribution of the misfit stress versus the distance the edge has been obtained and using finite element method in ref. [53]. Extension of the equilibrium theory of the critical thickness for the epitaxial layers suggested in ref. [54] is based on the proper account of the multiple reflection of the image dislocations.

3 Evolution of dislocation system

In thick ($h > h_c$) semiconductor layers grown at low temperatures the concentration of misfit dislocations is much smaller than that predicted by the thermodynamic equilibrium condition. Therefore the layers are metastable. When the metastable layers are heated at higher temperatures or during the continuous growth of the layers, dislocations are introduced and the strain relaxes. Generation of dislocations involves nucleation and/or multiplication and the glide motion of the dislocations. The creation of the misfit dislocations by multiplication also involves the glide of the dislocations and the nature of the dislocations depends on the growth mechanism of the layer.

At high temperatures, the growth mode is by three dimensional island growth because the atoms can more easily migrate to the islands. 3D growth mode is also occurs in the high lattice mismatch growth. In SiGe system with Ge content over 0.8 three growth stages have been observed [55]: 1) the pseudomorphic growth of thick (3-5 ML) wetting layer; 2) nucleation and growth of 3D islands; 3) coalescence of islands and continuos film growth. Misfit dislocations are readily nucleated at the boundaries between the islands [56].

To develop a model of strain relaxation through the system of dislocations, it is necessary to describe the dislocation motion and the evolution of the dislocation density due to their primary generation (misfit dislocation forming due the motion of existing threading dislocation, homogeneos and/or heterogeneous nucleation), multiplication, and interactions between dislocations (blocking, mutual fusion and annihilation) as well as with the native and artificially induced (such as cavities produced by He or H implantation and annealing [57, 58, 59]) defects. Development of the dislocation system in the substrate, generally speaking, should also be taken into account, since the

dislocation half-loops in the substrate could produce a great number of intersections in the glide planes [60]. Evidently, the detailed description of the strain relaxation in the heterostructures is extremely complex and, probably, excessive for the practical aim of optimization of the growth process.

3.1 Propagation of dislocations

The propagation of dislocations at low temperatures is dominated by a glide; a climb component that implies mass transport by diffusion in the bulk is significant at high temperatures only [61]. Velocities of the dislocations of different types can vary greatly. The thermally activated dislocation velocity is given by the equation

$$v_d = v_0 (\sigma_{\text{exc}})^m \exp(-E_v/kT) \tag{3}$$

where v_0 is a constant, σ_{exc} is the excess stress and E_v is the energy of activation for the glide motion of the dislocation, m usually taken as 1 or 2. The excess stress can be written as

$$\sigma_{\text{exc}} = 2S\mu\frac{1+\nu}{1-\nu}\varepsilon - \frac{\mu b\cos(\alpha)(1-\nu\cos^2\beta)}{4\pi h(1-\nu)}\ln\frac{\varrho h}{b} \tag{4}$$

where S is the Schmid factor. The first term in Eq. (4) is the stress acting on the dislocation line due to misfit strain and the second term is the self-stress of the dislocation line [62].

The stress σ_{exc} in the capped layers (strained buried layers) is as follows [61, 63]

$$\sigma_{\text{exc}} = 2S\mu\frac{1+\nu}{1-\nu}\varepsilon - \frac{\mu b\cos(\alpha)(1-\nu\cos^2\beta)}{4\pi h(1-\nu)}\ln\frac{\varrho h}{b} - \frac{\mu b\cos(\alpha)(1-\nu\cos^2\beta)}{4\pi h_{\text{eff}}(1-\nu)}\ln\frac{\varrho h}{b}$$

where

$$h_{\text{eff}} = \frac{hh_{\text{cap}}}{h+h_{\text{cap}}}$$

Evidently, both σ_{exc} and the velocity of the dislocation v_d are smaller in the capped layers. If the strained layer has an 'infinitely thick' capping layer $h_{\text{cap}} = \infty$, the self-energy of the dislocation line (dipole) increases by a factor 2 [64] and in the denominator of the second term in the eq. (4) "2" appears instead of "4".

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The velocity of dislocations in the different regions of a sample have been observed to be different by a factor up to 3 [65] due to the local variations of the stress.

The dislocation motion is usually described by the double (single) kink model. If the dislocation line is sufficiently long, several kinks may be formed at the same time. Single kinks are formed in the thin uncapped layers. As the layer thickness increases, the rate of nucleation of double kinks also increases. The transition thickness over which double kinks dominate has been estimated as 1 μm and 20 nm for the strains $\varepsilon = 0.2\%$ and $\varepsilon = 1\%$, respectively [66]. The activation energy is $E_v = E_m + F_k$ for single kink and $E_v = E_m + 2F_k$ for double kink models, where E_m is the activation energy for the kink jump along the dislocation line direction and F_k is the energy required to nucleate an isolated single kink.

The model [65] predicts the linear dependence of the velocity on the excess stress σ_{exc} and on the length of the dislocation length when the latter does not exceed a critical value.

The stability of the dislocation glide has been studied in ref. [67]. The kink motion in the field of random forces has been considered. It has been found that in the case of the low stress (compared to the Pierls stress) the attachment of the point defects to the dislocation core may cause both dislocation immobilization and instability of the dislocation glide. On the other hand, experimental data [68] show that the presence of the point defects could cause either increase or decrease of the dislocation velocity being dependent the defect nature, energy, concentration and the layer strain.

The authors of the cited paper have also studied the effect of the free surface on the dislocation propagation. While no systematic difference between measurement during growth and after growth has been registered, the dislocation velocity has been found to increase several times after forming a native oxide on the surface in the post-growth processing. The most possible explanation suggested in the paper is that the local stress at the oxide-layer interface can enhance kink nucleation rates at the surface.

The substrate thickness is finite, thus, there is strain of the opposite sign and much smaller in magnitude than in the epitaxial layer and threading dislocation in the substrate move in the opposite direction. As a result a "hairpin" configuration is formed. It consists of two long arms parallel to the surface (one at the interface, the other deep in the substrate), connected by a small threading segment [70].

3.2 Nucleation of dislocations

If the substrate is characterized by a sufficiently high density of the pre-existing threading dislocations, the necessary for the strain relaxation misfit dislocations are produced by the propagation of the threading segments. When the high quality substrates with the low dislocation density are used, the strain relaxation could be limited by the misfit dislocation generation.

Possible sources of misfit dislocations are:

- homogeneous nucleation of half-loops (whole or partial) at the free surface of the epitaxial layer

- homogeneous nucleation of half-loops at the substrate/epilayer interface

- heterogeneous nucleation of complete loops at the nucleation sites in the bulk of the epilayer

- heterogeneous nucleation of half-loops at the nucleation sites (point defects at the interface, edges of the islands

- multiplication of dislocations

The homogeneous nucleation of the dislocation half-loops at the surface of the semiconductor strained layers can be analysed through the behaviour of the total energy of the loop [66]

$$E^{\text{tot}} = E^{\text{loop}} - E^{\text{strain}} \pm E^{\text{step}} + E^{\text{fault}}$$

where E^{tot} is the self-energy of the semicircular loop of radius R, E^{strain} is the reduction of the homogeneous strain energy due to the interaction between the loop and the misfit strain and $E^{\text{step}} = 2Rs\gamma$ is the energy of the surface step which is necessarily created ($s = 1$) or destroyed ($s = -1$) if the Burgers vector of the dislocation has a vertical (normal to the surface) component. The last term $E^{\text{fault}} = \tilde{\sigma}^{\text{fault}}(h/\cos\alpha)$ is included in the case of a partial dislocation only [23]. It represents the energy of the stacking fault or the antiphase boundary created by the dislocation.

The total energy of the loop increases from 0 for $R = 0$ to a maximum value E^{act}, the activation energy for nucleation (which decreases with increase of the misfit f_m). The maximum occurs when $dE^{\text{tot}}/dR = 0$ at $R = R_c$, the critical radius of the loop. As the radius increases beyond R_c, the loop

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energy decreases and the loop grows at a rate determined by the velocity of the dislocations until it reaches the interface. After this, its threading segments move apart extending the misfit dislocation at the interface. The critical loop radius and corresponding activation energy are determined by [23]

$$R_c = \frac{B(1-\nu)(1-\frac{\nu}{2})b^2\left(1+\ln\left(\frac{\varrho R_c}{b}\right)\right) + 16(1-\nu^2)s\gamma}{8\pi(1-\nu^2)(\sigma b \sin\beta \sin\alpha \cos\alpha - E^{\text{fault}})}$$

$$E^{\text{act}} = R_c s\gamma + \frac{BR_c(1-\nu)(1-\frac{\nu}{2})b^2\left(\ln\left(\frac{\varrho R_c}{b}\right)-1\right)}{16(1-\nu^2)}$$

If the step and stacking fault energies as well as the logarithmic factors are neglected, it can be seen that $E^{\text{act}} \propto b^3$, i.e. it is easier to nucleate partial dislocations that have smaller Burgers vectors.

The rate of nucleation is generally assumed to be proportional to $\exp(E^{\text{act}}/kT)$. The estimates show that values of E^{act} are extremely high and thus homogeneous nucleation is very unlikely to occur for the reasonable values of the misfit parameter [66]. In most cases the observed values of the activation energies are much lower and have been attributed to the heterogeneous nucleation. It has been known for many years that point defects and their clusters lower the activation energy dramatically [33] and act as efficient sources for the nucleation of dislocations. Deliberate control of the number of these sources (by growing an intermediate layer with the high density of defects or introducing defects into the substrate) is widely used in practice [71] and presents an alternative to the classical layer grading [72].

The authors of ref. [73] argued that E^{act} in GeSi alloys should be lowered for the following reasons:

- preferential accumulation of Ge near the core in the compressed layers can substantially reduce the nonelastic core energy

- random fluctuation of Ge concentration results in the activation energy reduction in the regions where local Ge concentration is high

In [74] a regenerative source called 'diamond defect' with the low activation energy is described which is probably a result of the interstitial precipitation. Nucleation at the atomic ledges trapped at the interface between the substrate and the epitaxial layer has been suggested in ref. [75]. Unfortunately,

little theoretical work on the heterogeneous nucleation in the semiconductor strained layers has been done, presumably because many unknowns are involved and the process is very complex.

The modulation of the free surface (surface roughening) can provide regions (ripple throughs) of the large stress where the activation barrier for dislocation nucleation is extremely low [76]. It has been shown that its value is proportional to ε^{-4} while for the dislocation nucleation by other mechanisms usually varies as ε^{-1} [77]. Thus nucleation of dislocations via surface roughening dominates for the large values of f_m.

Note that the half-loop can nucleate at the surface only if $h \geq h_d$, where $d = R_c \cos\varphi$, φ is the angle between the surface and the normal to the slip plane.

3.3 Multiplication of dislocations

The most popular mechanism invoked for the multiplication of dislocations is the well-known Frank-Read source or its modification. A characteristic feature of this mechanism is that often the large dislocation loops extended into the Si substrate as well as the dislocation pile-ups several microns deep are observed [77]. Another multiplication process is the so-called Hagen-Strunk mechanism [78] that operates when two dislocations meet each other at the right angle. Multiplication of dislocations by this mechanism has been observed in both GeSi [74] and InGaAs [79] strained layers. It operates efficiently, however, only if neither the layer thickness nor the misfit are large. There are also doubts of the correctness of observations interpretation as Hagen-Strunk mechanism in some cases [80]. Both Frank-Read nad Hagen-Strunk mechanisms lead to the bunching of the dislocations with identical Burgers vectors. Filling the area between this bunches could be promoted by the cross slip process [69, 70].

The rate of multiplication is commonly written as

$$\left(\frac{dN}{dt}\right)_{\text{mult}} = K N_m v_d \tag{5}$$

where K is a breeding factor and N_m is the number of mobile threading dislocations. A breeding factor is usually considered to be either constant [66] $K = K_0$ or proportional to the excess stress [81] $K \propto \sigma_{\text{exc}}$.

A more elaborate expression has been suggested for the Hagen-Strunk

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multiplication mechanism [66]

$$\left(\frac{dN}{dt}\right)_{\text{mult}} = -\frac{(f_m + \varepsilon)N_m v_d}{2b_{\text{eff}}}P_{\text{mult}} \tag{6}$$

where P_{mult} is the probability that an interaction of the appropriate type leads to a multiplication event that depends on the lattice mismatch and the thickness of the layer.

3.4 Interaction of dislocations

Dislocation interactions not only influence the rate at which the dislocations propagate, but also can halt the threading dislocation motion entirely. Additionally, blocked dislocations can alter the surface morphology as well as limit the overall relaxation of technologically important low-dislocation-density, graded buffer structures. On the other hand, annihilation of the threading segments could lead to the significant reduction of the dislocation density in the strained layer.

3.4.1 Blocking (pinning) of dislocations

Two blocking mechanisms are known. The first one, *long-range blocking*, has been described over a decade ago [22]. Recently another blocking mechanism named *reactive blocking* has been detected both experimentally (by real time transmission electron microscopy observations) and numerically (using discrete disclocation dynamics computations of the strained layer relaxation) [83].

3.4.1.1 Long-range blocking The misfit dislocation could impede the motion of the threading dislocation if the two dislocations have the right kind of Burgers vectors. There are four pairs of strain relieving Burgers vectors, only one of which causes the significant blocking of the moving dislocation. The probability that the dislocation interaction can impede the motion of the threading dislocation is therefore 1/4.

As a propagating threading dislocation approaches an interfacial misfit dislocation segment, the strain fields associated with each dislocation begin to overlap, resulting in an interaction force that has the general form:

$$\sigma_{\text{int}} \propto \frac{\mathbf{b_1} \cdot \mathbf{b_2}}{r}$$

where $\mathbf{b_1}$ and $\mathbf{b_1}$ are the Burgers vectors of the two dislocations and r is the distance between them. Thus, this force can act to either increase or decrease the magnitude of the net stress that drives the threading dislocation forward, depending on the signs of the Burgers vectors of the dislocations involved. If this interaction stress cancels the other stresses over a significant portion of the threading segment, the motion of the entire dislocation will be halted. If the interaction stress is not sufficiently large, the threading dislocation will propagate past the misfit interfacial segment.

To bypass the blocking misfit dislocation, the threading dislocation should alter its path by moving in the same glide plane but closer to the free surface, i.e. in a channel of the width $h^\star$ smaller than the layer thichness. Three forces act on the threading dislocation in this configuration:

1. the driving force due to the residual homogeneous strain

2. the retaining force due to the line tension of the threading dislocation (including the interaction with the surface via the image forces

3. the interaction force with the misfit dislocation

The condition of blocking the threading dislocation motion could be written as an equation for critical value of $h^\star$ [84]

$$\varepsilon - \varepsilon_r = \frac{3b}{16\pi h^\star(1+\nu)}\left(\frac{4-\nu}{3}\ln\left(\frac{8h^\star}{b}\right) - \frac{1}{2}\cos(\alpha) - \frac{1-2\nu}{4(1-\nu)}\right),$$

where ε_r is the reduced strain due to the presence of misfit dislocation.

The described blocking mechanism is enhanced due to the presence of the surface ripples as result of the stress field of the orthogonal misfit dislocation [85, 86] and could lead to the threading dislocations pile-ups to be discussed later in this section.

3.4.1.2 Reactive blocking A new strong blocking effect observed using real time TEM has been studied by numerical simulations [83]. A propagation of the threading segment towards the misfit dislocation on an intersecting glide plane has been analysed. With the available Burgers vectors and directions of approach, sixteen distinct interactions of this kind are possible, leading to a variety of outcomes such as repulsion of the misfit dislocation into the substrate, reconnection of the two dislocations, and junction or jog creation. It was found that four of the interactions involve the parallel Burgers vectors

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and can result in a reconnection reaction. The authors claim that this blocking mechanism is much stronger than the conventional (long range) misfit-blocking interaction. Unfortunately, no analytical model/approximation is proposed in the paper.

3.4.1.3 Overall blocking effect   The number of dislocations blocked per unit time is defined as [66]

$$\left(\frac{dN}{dt}\right)_{\text{block}} = \frac{dN_i(t)}{dt}P(t) \tag{7}$$

where $N_i(t)$ is the total number of interactions and P (t) is the blocking probability. P (t) is 1/4 if the blocking occur (the local force is greater than the critical value) and zero otherwise. Eq. (7) could be re-written as

$$\left(\frac{dN}{dt}\right)_{\text{block}} = -\frac{(f_m + \varepsilon)N_m v_d}{2b_{\text{eff}}}P(t)$$

If the propagating threading dislocation interacts with a closely bunched cluster of N misfit dislocations with the identical Burgers vectors, the interaction force is multiplied by a factor N [82].

The pile-up formation mentioned above could be responsible for the strain (work) hardening [87] and observed slowing of strain relaxation in the layer at the late stages. An indirect confirmation of the importance of the pile-ups formation in SiGe is the effect of the chemical-mechanical polishing at the intermediate growth stages on the final threading dislocation density reduction [88]. It is believed that planarization of the surface free the threading dislocations pinned in the pile-ups.

Introduction of hardening is a way to account integrally for the numerious interactions between the dislocations. While on atomic level plastic flow is always very inhomogeous, its macroscopic phenomenological description via the flow stress

$$\tau = \alpha_\tau \mu b \sqrt{\rho}$$

where the coefficient α_τ depends on the strain rate and the temperature is commonly used and proved to be reasonable for most cases of strain hardening in a wide range of materials [89].

Table 1: Basic binary reactions between threading dislocations

2nd plane	$(b_2)_z$	Treading	Misfit
111	positive	fusion	single line
111	negative	annihilation	single line
1$\tilde{1}$1	positive	fusion	two-arm
1$\tilde{1}$1	negative	annihilation	two-arm

3.4.2 Fusion and annihilation of dislocations

The outcome of the binary reaction of two threading dislocations depends on the relative arrangement of their gliding plabes and the orientation of the Burgers vectors. Possible cases including fusion and annihilation of dislocations have been considered in ref. [70]. Assuming that the first threading dislocation propagates in the plane (111) and its Burgers vector $\mathbf{b}_1$ has a positive projection on the vertical direction, basic binary reactions are summarized in the Table 1. The critical parameter for these reactions is the interaction radius. A continuum-based approach using linear elasticity has been employed to compute this variable for the dislocations in the heteroepitaxial system in ref. [90]

4 Strain relaxation models

4.1 Discrete models

A number of both micro- and mesoscale numerical models [91] have been applied to the study of the relaxation mechanisms of the strained epitaxial layers.

4.1.1 Atomistic models

First-principles total energy computations has been used to resolve the disagreement of the experimentally determined relation between lattice relaxation in in-plane and out-of-plane directions with the predictions of classical elasticity [92]. It was found that segregation at the interface significantly influence strain relaxation in the heterostructure.

The deformation state of the heteroepitaxial strained system has been

studied using atomistic simulations in [93, 94]. A three-step relaxation procedure has been developed:

1. structural relaxation with composition being fixed

2. compositional relaxation

3. further local structural relaxation

Conjugate gradients method has been used for the energy minimization at the first and third stages while Metropolis implementation of Monte Carlo method has been applied to the compositional relaxation.

Molecular dynamics simulations have been used in ref. [40] to capture the growth process at the atomic level and to study the mechanisms of the dislocation formation. The embedded atom method has been employed that in addition to the binary interactions efficiently accounts for the many-body effects. The kinetic constrained influence on the atomic assembly process has been studied.

In ref. [95] the two-dimensional Frenkel-Kontorova model has been applied to computation of the dislocation nucleation rate in the growing heteroepitaxial island. As in the preceding paper, the embedded atom method has been used to compute the total energy.

One-dimensional Monte Carlo method has been used to simulate the surface height evolution during and after the strain relaxation in ref. [96]. The aim of this study was to get insight into the cross-hatch morhology development and to asses different existing models of the process (such as enhanced growth over strain relaxed regions due to the lateral transport by surface diffusion and surface undulations caused by the dislocation generation and glide). The authors conclude that surface step flow is a necessary condition for the development of the mesoscale cross-hatch morphology while the plastic relaxation itself could not produce the undulations of significant amplitude.

4.1.2   Mesoscopic models

Detailed simulations of the interaction of the two threading segments encountering each other in a thin strained SiGe layer has been performed in ref. [97] using the full three-dimensional Peach-Koehler formalism [98]. The force acting on a dislocation segmeny $d\mathbf{l}$ in the glide plane is

$$b_i \sigma_{ij} n_j (\mathbf{n} \times d\mathbf{l})$$

where **n** is the normal to the glide plane. The stress tensor includes stresses due to the applied strain and stresses generated by the presence of dislocations. The authors have avoided the difficulties with the stress correction caused by the presence of surfaces by considering the symmetrically capped layer.

In a few recent papers [83, 99, 100, 101] the application of the discrete dislocation dynamics method to the strain relaxation has been reported. Large scale 2D simulations are used to study the misfit strain relaxation in the hetroepitaxial islands in ref. [99], pecularities of the hardening in the single crystal thin films has been investigated in ref. [100]. Monitoring of the evolution of a few hundreds dislocations in the strained layer [83, 101] leaded to a discovery of a new blocking mechanism discussed briefly in the preceeding section.

4.2 Continuum models

A classification of continuum (macroscopic) models adopted below is by no means unique and generally accepted. Still, it is worth to make an attempt to sort out different approaches to the simulation of the strain relaxation. The main problem is, of course, a considerable overlapping of ideas and methods.

4.2.1 Equilibrium models

4.2.1.1 Uniform layer The equilibrium density of the misfit dislocation in the strained layer with the uniform composition is obtained similar to the analysis of the critical thickness by the energy minimization [61]. A coarse estimate of the threading dislocation density as 1-2 times that for misfit dislocation follows from the scheme of the misfit dislocation generation due to the threading segment motion ($\rho_{\mathrm{td}} = \rho_{\mathrm{md}}$) or by half-loop nucleation ($\rho_{\mathrm{td}} = 2\rho_{\mathrm{md}}$). These estimates, of course, do not account for the threading dislocation density reduction due to the fusion/annihilation.

An estimate for the threading dislocation density via the average misfit dislocation length has been suggested in ref. [103], assuming that two threading dislocation are connected by a misfit segment with lenghth $\langle l \rangle$. Similar relation has been suggested later [104]:

$$\rho_{td} \approx 4\rho_{md} \left(\frac{1}{\langle l \rangle} - \frac{1}{L} \right)$$

where L is the sample size and ρ_{md} is determined via the lattice mismatch.

A model for the equilibrium threading dislocation density in the thick layer (compared to the critical thickness) has been analysed in [105] with neglection of the misfit strain. The author assumes that the population of the threading dislocations is governed by the coalescence of the close dislocations and introduces the 'minimum stable separation' (i.e. the fusion/annihilation radius) estimated as

$$\frac{1}{r_{\min}} = \frac{\cos\phi}{4h}\left(\cos^2\beta + \frac{\sin^2\beta}{4(1-\nu)}\ln\left(\frac{\sin\alpha\sin\beta}{4f_m}\right)\right)$$

Then $\rho_{\mathrm{td}} = 2/(R_{\mathrm{av}}r_{\mathrm{av}})$ where R_{av} is the average spacing between the glide planes defined by the misfit and $r_{\mathrm{av}} = 2r_{\min}$ is the average distance between the threading dislocations within the plane. The model reasonably predict both the mismatch dependence and the order of magnitude of the threading dislocation density for some materials in the range $f_m = 0.002 - 0.1$. Still, the author, being aware of the simplifications made, lists major of them: 1) the large layer thickness $h \gg h_c$; 2) approximations in the line tension calculations; 2) assumed large spacing of the misfit dislocations; 4) no kinetic barriers to the glide of the threading dislocations; 5) the threading dislocations density is considered as a function of the film thickness only, while experiments show that it varies across the layer.

The author also notes that the difference between the strain accomodation by 60° misfit dislocations and the pure edge ones (a factor 2 in the threading dislocation density) explaines the twofold reduction of the dislocation density in some materials during the post-growth annealing by transformation of the first type dislocations into the second one.

4.2.1.2 Graded layer Strain relaxation in the linear graded epitaxial layers has been considered in ref. [106]. The term "equilibrium dynamics" used by the authors is somewhat misleading. In fact a quasi-stationary approach is exploited. A set of algebraic equations that define the current values of the lattice constant, strain, biaxial modulus and shear modulus as a function of the film thickness is formulated. Expressions for the local relaxation thickness h_c^l, the plastic strain and the equilibrium dislocation density are obtained. The value of h_c^l is attributed to the size of the dislocation-free region on the top of the growing layer. Its predicted weak dependence on the film thickness as well as the strong effect of the grading rate on both the local

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relaxation thickness and the equilibrium disclocation spacing are confirmed by the experimental data.

The influence of the grading law on the residual strain, the threading dislocation and misfit dislocation density has been studied theoretically and experimentally in ref. [107]. The authors assume that the grading, however, does not change the basic phenomena such as nucleation/multiplication studied in detail for the uniform layers. The standard relation between the strain and the misfit dislocation density is generalized to

$$\varepsilon(h) = -f_m(h) + b_\| \int_0^{h_f} \rho_{\mathrm{md}} dh$$

where $\varepsilon(h)$ and $f_m(h)$ are the depth profiles of the residual strain and of the lattice misfit, respectively, h_f is the total film thickness. Assuming full relaxation, the authors get

$$\rho_{\mathrm{md}} = \frac{1}{b_\|} \frac{d}{dh} f_m(h)$$

Accounting for the existence of the top dislocation-free layer of the thickness h_c, the residual strain distribution is written as

$$\varepsilon(h) = \begin{cases} 0, & if \quad 0 \le h \le h_f - h_c \\ -(f_m(h) - f_m(h_f)), & if \quad h_f - h_c < h \le h_f \end{cases} \quad (8)$$

Several layers with different grading laws (linear, parabolic, square-root, step + linear) have been grown. The analysis of the observed work hardening forced the following modification of eq. (8):

$$\varepsilon(h) = \begin{cases} \varepsilon^{\mathrm{wh}}(h), & if \quad 0 \le h \le h^{\mathrm{wh}} \\ -(f_m(h) - f_m(h^{\mathrm{wh}}) - \varepsilon^{\mathrm{wh}}(h)), & if \quad h^{\mathrm{wh}} < h \le h_f \end{cases}$$

where the supersript 'wh' refers to workhardening and, as experiments show, $h^{\mathrm{wh}} > h_f - h_c$.

4.2.2 Reaction kinetics models

An evolutionary approch based on *reaction* and *reaction-diffusion* models has been applied to a number of the misfit strain relaxation problems. A

general form of kinetics equations used to study the threading dislocation reduction in the strained layers is as follows [108]-[111]

$$\frac{d\rho_i}{dh} = -\sum_j K_{ij}\rho_i\rho_j + \sum_l \sum_m K_{lm}\rho_l\rho_m \qquad (9)$$

where ρ_i is the density of the specific i^{th} dislocation family and the kinetic coefficients K_{ij} are the rates of the reactions between the dislocations from the families i and j. These equations described the dislocation densities evolution

- with the layer thickness during growth $\rho_i = \rho_i(h)$ or

- in time for the film of the fixed thickness $\rho_i = \rho_i(t)$

Both first- and second order reactions could be considered (the order of a reaction corresponds to the number of participants). For example, blocking of the threading dislocation propagation due to the interaction with the misfit dislocation is the first-order reaction while both fusion ($\mathbf{b}_3 = \mathbf{b}_1 + \mathbf{b}_2$) and annihilation ($0 = \mathbf{b}_1 + \mathbf{b}_2$) are the second-order reactions.

The complete treatment of the strain relaxation using the reaction equations requires the account of the crystallographic details and a subdivision of the dislocation system into separate populations corresponding to the specific Burgers vectors and line directions. For f.c.c. semiconductors, for example, there are 24 dislocation sets arising from the combination of four possible (111) type slip planes and six Burgers vectors; 20 families of dislocations in GaN have been considered in ref. [111].

The coupled system of nonlinear ODEs being rather complex, reduced models are frequently used. An obvious bonus of the model reduction is the possibility to obtain an analytical solution for some limiting cases [108, 110].

For example, in the model of ref. [112] misfit dislocations are created exclusively by lateral bending of the threading segments and threading dislocations by half-loop nucleation at the surface at rate j; threading dislocations are blocked by the misfit ones with the probability η and multiplication is neglected. Thus the following system is used

$$\begin{aligned}
\frac{\partial \rho_{md}}{\partial t} &= v\rho_{td} \qquad (10) \\
\frac{\partial \rho_{td}}{\partial t} &= j - \eta v \rho_{td}\rho_{md}
\end{aligned}$$

The review of some early reaction type models has been given in [105]. The first one ("annihilation-coalescence" model) is just an equation for the total dislocation density that accounts for the fusion and annihilation of dislocations

$$\frac{d\rho}{dh} = -A\rho - B\rho^2$$

leading to the relation

$$\rho(h) = \frac{1}{\left(\dfrac{1}{\rho_0} + \dfrac{B}{A}\right)\exp(Ah) - \dfrac{B}{A}}$$

The "half-loop" model based on the assumption that the fusion of the threading dislocations results in the formation of half-loops and half-loops smaller than a certain critical size are removed from the layer by gliding to the interface leads to the following equation for the total dislocation density

$$\rho = \frac{f_m\sqrt{2}(1-\nu)(1-2\nu)\ln\left(\dfrac{2\pi f_m}{1-\nu}\right)}{bh(1-\nu)^3(1-\ln(2b\sqrt{\rho}))}$$

The set containing three dislocation families (mobile and immobile threading dislocation; misfit dislocation) has been exploited in ref. [110] and extended in ref. [113] to the four unknowns system by splitting the population of the misfit dislocations into an 'active' and a 'passive' parts. Analytic solutions have been obtained for a number of special cases (no blocking of the threading dislocation propagation by the misfit dislocation or no annihilation reaction). Eqs. (9) is used to study the dislocation evolution either in the layer of the fixed thickness or during the growth, i.e. for the single independent unknown.

Dislocation densities of the gliding and climbing threading dislocations as well as of the misfit dislocations has been considered in ref. [114]. The authors stress the importance of the climb process inclusion into the model since it permits the description of the effect of point defects on the dislocation propagation.

Another feature of this model is the attempt to account for the nonlocal character of the threading dislocation interaction with the misfit dislocation by introducing the diffusion term into the conservation equation for the

gliding dislocation density. The principal character of this extension is the transition from ODE to PDE:

$$
\begin{aligned}
\frac{\partial \rho_g}{\partial t} &= A\sigma(z) - B(\rho_g)\rho_g + D\frac{\partial^2 \rho_g}{\partial z^2} \qquad (11)\\
\frac{\partial \rho_c}{\partial t} &= B(\rho_g)\rho_g - K\rho_c \\
\frac{\partial \rho_m}{\partial t} &= K\rho_c
\end{aligned}
$$

where ρ_i, $i = g, c, m$ are the density of the gliding, climbing and misfit dislocations, respectively, A, B, K - corresponding reaction rates [114, 115].

The model just described has been applied to the problem of the misfit dislocation patterning [115, 116]. The complete system has been used for the linear stability analysis only, while dislocation evolution has been considered for the two limiting cases: the uniform time-dependent solution $\rho_i = \rho_i(t)$ and the steady-state non-uniform one $\rho_i = \rho_i(z)$.

4.2.3 Plastic flow models

Phenomenological plastic flow models of the dislocation evolution are based on the well-known Alexander-Haasen (AH) model [117] developed for elemental semiconductors loaded in a single slip orientation. It uses the dislocation density as a state variable and relates the plastic deformation in the crystal to the movement and multiplication of dislocations. Usually under AH model (or Alexander-Haasen-Sumino model) a tuple of three components is meant [118]. These components are:

1. Orowan equation [119] that relates the plastic shear strain rate to the motion of mobile dislocations

$$\dot{\varepsilon}^{\text{pl}} = Nbv_d$$

2. normalized expression for the dislocation velocity eq. (3) with a substitution σ_{eff} instead of σ_{exc}

$$v_d = v_0 \left(\frac{\sigma_{\text{eff}}}{\sigma_0}\right)^m \exp\left(-\frac{E_v}{kT}\right)$$

3. equation for the dislocation density evolution

$$\dot{N} = \delta N v_d$$

The main contribution to the model by Alexander and Haasen themselves is the adaptation of the relation for the dislocation velocity to the case of covalent crystals with high Peierl barrier. They gave an explanation to the Arrhenius type temperature dependence of the dislocation velocity observed in experiments, in particular, in Ge [120]. To determine the backstress $\hat{\sigma}$ in

$$\sigma_{\text{eff}} = \sigma_{\text{exc}} - \hat{\sigma}$$

the authors consider a statistical arrangement of N parallel dislocations giving the backstress

$$\hat{\sigma} = \frac{\mu b}{2\pi(1 - \nu)} N^{1/2}$$

that is consistent with the square-root dependence suggested by G.I. Taylor.

The multiplication law is due to Johnson & Gilman [121]. Alexander and Haasen postulated that the breeding coefficient is

$$\delta = K\sigma_{\text{eff}}$$

where K is an empirical constant.

Refs. [81, 63, 122] are probably the first examples of the application of AH-type models to the strain relaxation in the thin films. The main modification of the plastic flow model in the first of the cited papers is an analysis of both gliding and climbing dislocation motion resulting in the equation for $\gamma = f_m - \varepsilon$

$$\frac{d\gamma}{dt} = \frac{\sigma_{\text{eff}}^2}{\mu^2} \left(\Gamma_g \exp{-\frac{E_g}{kt}} + \Gamma_c \exp{-\frac{E_c}{kt}} \right) (\gamma + \gamma_0)$$

or

$$\frac{d\ln(\gamma + \gamma_0)}{dt} = \frac{\sigma_{\text{eff}}^2}{\mu^2} \left(\Gamma_g \exp{-\frac{E_g}{kt}} + \Gamma_c \exp{-\frac{E_c}{kt}} \right)$$

where Γ_g and Γ_c are the glide and climb prefactors, respectively, E_g and E_c are the activation energies and γ_0 represents a "source" term needed for starting multiplication process. As noted in [61], in the more accurate formulation the excess in-plane stress should be replaced by the excess stress resolved on the slip plane. To adjust Γ_g, Γ_c, E_g, E_c and γ_0, experimental data [123, 124] have been used.

The essence of the 'improved' Dodson-Tsao model proposed in [66] is the account for different processes that change the dislocation density

$$\frac{dN}{dt} = -Q_{\text{block}} + Q_{\text{nucl}} + Q_{\text{mult}}$$

In ref. [125] AH-type model has been applied to the strain relaxation in the graded SiGe layer. Under a number of simplifying assumptions the authors get an expression for time derivative of the dislocation density that depends linearly on both the growth rate R_g and the grading rate R_{gr}

$$\frac{d\rho}{dt} \propto R_g R_{gr}$$

Clearly, this relation does not endure the limiting transition to the case of the uniform layer growth.

In the investigation of the strain relaxation in the uniform layer [126] σ_{eff} has been used in the equations for both the dislocation velocity and dislocation density evolution. However, the backstress has been determined as

$$\hat{\sigma} = BH(\varepsilon^{\text{pl}}) = B\alpha \left(\frac{\varepsilon^{\text{pl}}}{f_m} \right)^{\beta} \left(1 - \tanh \frac{\gamma \varepsilon^{\text{pl}}}{f_m} \right) \tag{12}$$

where α, β, γ are ajustable parameters.

This model has been extended to the case of multiple and graded layers in ref. [127]. The source term in the equation for the dislocation density evolution has been separated into nucleation and annihilation parts

$$\dot{\rho} = \dot{\rho}_{\text{nucl}} + \dot{\rho}_{\text{annih}}$$

A threshold stress for the threading dislocation nucleation σ_0 has also been introduced

$$\dot{\rho}_{\text{nucl}} = \xi_0 \left(\frac{\sigma_{\text{exc}} - \hat{\sigma} - \sigma_0}{\mu} \right) \exp - \frac{E_\rho}{kT}$$

The autors assume that dislocation multiplication plays a relatively minor role; the threading dislocations nucleate at the surface and distributed to all the layers according to some weight - a power function of the effective stress has been adopted in the paper.

An extension of the Dodson-Tsao model [81] suggested in ref. [128] is mainly a modification of the rate equation for the surface nucleation. In addition to the nculeation equation itself

$$\frac{d\rho}{dt} = \xi_0 \left(\frac{\sigma_{\text{eff}}}{\mu} \right)^{(1+\alpha)} N_s$$

an equation for the time evolution of the nucleation site density N_s is introduced

$$\frac{dN_s}{dt} = G - \frac{N_s}{t_0}$$

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where t_0 is the characteristic time of the source deactivation. This modification seems to be specific for III-V heterostructure growth where, in contrast to the SiGe material system, a significant reduction of the strain relaxation rate at the growth interruption is observed. The extended models gives the deviation from the experimental data twice smaller than the model [81].

The AH-type model has been used to study the strain relaxation in the structure with the substrate of finite thickness in the multiscale approach of ref. [94]. The model equations have been combined [129, 130] with the equation of the mechanical equilibrium

$$M_f \varepsilon_f h_f + M_s \varepsilon_s h_s = 0$$

and the compatibility equation

$$\varepsilon_f - \varepsilon_s = f_m - sbN_{md}$$

where

$$s = \left\{ \begin{array}{ccc} 1 & for\ tensile\ strain & f_m > 0 \\ -1 & for\ compressive\ strain & f_m < 0 \end{array} \right.$$

to get an ODE for the single unknown - the strain in the layer ε_f - as a function of the film thickness [94, 130].

5   Conclusions

5.1   Strain relaxation scenario

The overall scenario of the strain relaxation in the heteroepitaxial structure with low/medium lattice mismatch includes the following stages:

1. elastic strain accomodation

2. slow strain relaxation

3. fast strain relaxation

4. relaxation saturation due to strain hardening

An additional process to be considered is the relaxation during the annealing. This stage is somewhat simpler in the numerical analysis since the film thickness is fixed.

5.2 Assessment of strain relaxation models

5.2.1 Discrete models

The advantage of the micro- and mesoscale numerical models of the misfit strain relaxation is the detailed description of the processes. There are, however, two drawbacks. The first one is evident: huge computer resources for the real-life problems. The second one is more subtle, but actually more severe: the need for corresponding initial and boundary conditions.

Thus, at the present time, such discrete numerical models could be practically usefull

- as a component of a multiscale simulation system either directly or via homogenization-type procedure

- as a measuring stick for the calibration of the continuum models [102]

5.2.2 Continuum models

It is evident that estimate of the dislocation density using equlibrium models will always produce an *upper* bound of this parameter and a *lower* bound for the residulal strain.

Reaction and reaction diffusion models allow a detailed description of the interaction of the dislocations belonging to the different slip systems. Their weak point is first of all the absence of a mechanism to account for the collective behaviour of the dislocations and its effect on the strain. The known applications of the models of this kind deal with either of

- dislocation evolution versus the film thickness

- with annealing of the constant thickness film

The reaction-diffusion models described above that include the gradient terms are formulated as two dimensional problems. The spatial coordinate is in-plane, however, and solutions published are either uniform (zero spatial dimension) non-stationary or 1D stationary.

Plastic flow models relay heavily on the tuning to the experimental data. Still, it seems that at present they are capable to account best (phenomenologically) for the complex processes of the strain relaxation in the heterostrucures, provided enough experimental information is available for the reliable

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determination of the adjustable parameters. In the all known examples plastic flow models used for the relaxation during growth are written in terms of the layer thickness as an independent variable. These models have been also applied to the simulation annealing.

5.3   Evolutionary model

The comprehensive model of misfit accomodation should describe the strain relaxation and the dislocation evolution both during the growth itself and the post-processing (annealing). As the first step we are considering the layer only without the substrate.

The model for the strain relaxation in the heterostructure being implemented now is an adaptation of the model developed for the analysis of dislocation density evolution during the growth of single bulk crystals [131]. Its major features are as follows.

The strain is divided into elastic and plastic components:

$$\varepsilon_{ik} = \varepsilon_{ik}^{el} + \varepsilon_{ik}^{\mathrm{pl}}$$

Strain is related to the stress via Hooke's equation which in general case of anysotropic crystal can be written as

$$\sigma_{ik} = \sigma_{ik}^{el} + c_{iklm}(\varepsilon_{lm}^{\mathrm{pl}} - \beta_{lm}\triangle T)$$

where σ_{ik} is the stress for completely elastic case which should be used in the equilibrium equations, σ_{ik}^{el} is the real elastic stress, $\triangle T$ is relative temperature, c_{iklm} are elastic constants and β_{ik} are thermal expansion coefficients, which are usually assumed to be isotropic: $\beta_{ik} = \delta_{ik}\alpha$.

The dependence of the density of dislocations flux tensor on deviatoric stress is taken from [132]:

$$j_{ik} = -\frac{S_{ik}}{\sqrt{J_2^S}}bNv$$

where S_{ij} and J_2^S are the elastic deviatoric stress and it's second invariant, respectively:

$$S_{ik} = \sigma_{ik}^{el} - \frac{1}{3}\delta_{ik}\sigma_{ll}^{el}, \quad J_2^S = \frac{1}{2}S_{ik}S_{ik}$$

Using the generalization of the Orowan equation

$$\delta\varepsilon_{ik}^{\mathrm{pl}} = -\frac{1}{2}(j_{ik} + j_{ki})\delta t$$

one finally obtain

$$\frac{d\varepsilon_{ik}^{\text{pl}}}{dt} = \frac{S_{ik}}{\sqrt{J_2^S}}bNv \tag{13}$$

The equation for the total dislocation density and the dislocation velocity are written as

$$\frac{dN}{dt} = K\sigma_{eff_N}^{\lambda}Nv + \dot{N}_{bin}$$

$$v = v_0\sigma_{\text{eff}}^m sign(\sigma_{\text{eff}})\exp-\frac{Q_v}{kT}$$

where the term $\dot{N}_{bin}$ accounts for the binary dislocation reactions and K, λ, v_0, m, Q_v are the material parameters.

Effective stress is defined as

$$\sigma_{\text{eff}} = |\sigma - \xi\mu b\sqrt{N}|$$

σ is applied elastic stress and ξ is the strain hardening factor. A hardening function (12) is considered as a probable alternative.

The straightforward extension of the model is possible to account for the dislocation evolution along each slip system. However more accurate such model may appear, one should bear in mind that the number of the material parameters will blow up. For example, in the Orowan equation (13) bNv is to be changed to the sum over all slip systems [133]

$$\sum_i b_i N_i (v_d)_i$$

while the effective stress for the ith slip system should be written as [134]

$$(\sigma_{\text{eff}})_i = |\sigma_i - \xi_i\mu b_i\sqrt{N_i}| - \mu b_i\sqrt{(\sum_j(\chi_{ij}N_j))}$$

Thus it has been decided to start with the model for the evolution of the total dislocation density.

As has been mention already, all the models of the strain relaxation during the growth reviewed above (as well as most examples of the AH model applications to the density evolution in the bulk crystals, starting with the classical papers [135, 136]) are written as the equations in the layer thickness instead of time as an evolutionary variable. In other words, it is assumed

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that the dislocation motion is instantly frozen and no relaxation occur in the part of the layer that has been already grown. If it is probably acceptable for the growth of III-V thin films, it is certainly not true for the SiGe epitaxial growth: as experiments show, the growth interruption does not stop the relaxation process. The model outlined briefly in this section is a true transient one similar to the model used recently for the growth of bulk crystals [137]. Moreover, it allows the uniform treatment of the growth itself and annealing.

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