Semiconductors, Vol. 37, No. 5, 2003, pp. 493–518. Translated from Fizika i Tekhnika Poluprovodnikov, Vol. 37, No. 5, 2003, pp. 513–538.
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REVIEW

Artificial GeSi Substrates for Heteroepitaxy: Achievements and Problems

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Submitted October 22, 2002; accepted for publication November 30, 2002

Abstract—It is desirable to have a set of substrates which are based on Si and ensure growth of heterostructures with various lattice parameters in order to develop electronic devices composed of semiconductor materials whose epitaxial growth is reasonably well developed. Such substrates are typically referred to as artificial. In this paper, a comparative analysis of various methods for the fabrication of artificial substrates (heterostructures), in which the relaxation of stresses is based on the introduction of misfit dislocations, is performed. Based on published and new experimental data, the mechanisms for attaining a low density of threading dislocations in plastically relaxed films represented by heterostructures composed of GeSi and an Si buffer layer grown at low temperatures are analyzed. The problems and results of another group of methods for obtaining artificial substrates which gained favor recently and become known as "compliant" or "soft" substrates are discussed. The most important electrical parameters of Si and GeSi films grown on artificial substrates are considered. *© 2003 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

The term "artificial substrate" is used to denote a heterostructure that is grown epitaxially on an Si (or GaAs) substrate and has new valuable characteristics: a perfect crystal structure and surface smoothness which differ only slightly from those of the initial substrate; however, an artificial substrate differs radically from an initial substrate in its lattice parameter. Perfect heterostructures based on GeSi/Si make it possible to significantly improve the characteristics of devices produced conventionally on Si substrates (for details, see the reviews [1–3]). Another special feature of these heterostructures consists in the fact that they can be used as artificial substrates for the growth of GaAs, which could result in compatibility of the devices based on silicon technology with optoelectronic devices based mainly on GaAs. The most important components for ensuring this compatibility are Ge_xSi_{1-x} buffer layers, which make it possible to form completely relaxed, perfect layers of Ge–Si solid solution with x as large as unity; as a result, the formation of epitaxial Ge/Si structures with a low defect concentration becomes possible.

The physical mechanism which underlies the epitaxial transition of one material to another with differing lattice constants and is used in conventional methods consists in the relaxation of elastic strains in a thin layer of new material by introducing misfit dislocations (MDs). However, the introduction of MDs gives rise to so-called threading dislocations, which are dislocation-loop segments that emerge at the surface of an epitaxial layer. In order to reduce the density of threading dislocations, one conventionally uses either buffer layers with the lattice varying across the layers or so-called dislocation filters composed of stressed superlattices.

The main requirements imposed on the above substrates are (i) small thickness of the film in which plastic relaxation occurs; (ii) a perfect crystal structure, which is mainly assessed from the threading-dislocation density; and (iii) low roughness of the heterostructure surface.

Recently, a number of methods for the production of new artificial substrates referred to as "compliant" and "soft" ones have been suggested. When these substrates are used, it is assumed that a completely different physical mechanism is in effect: redistribution of stresses between the pseudomorphic layer and thin (compliant) substrate–membrane; as a result, the pseudomorphic layer relaxes elastically without the formation of MDs and, correspondingly, without generation of threading dislocations.

2. PLASTIC RELAXATION OF HETEROSTRUCTURES AS A CLASSICAL METHOD FOR THE FORMATION OF ARTIFICIAL SUBSTRATES

2.1. Basic Points of the Plastic-Relaxation Theory for Artificial Substrates

It is well known that plastic relaxation of mismatch stresses in GeSi/Si films is mainly attained by the introduction of 60° dislocations over the inclined {111} glide planes (see, for example, [3]). The initial stage of plastic relaxation of a pseudomorphic film is shown schematically in Fig. 1. The relaxation sets in with the

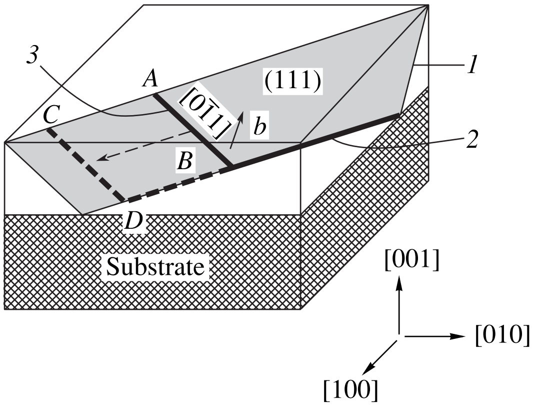


Fig. 1. Schematic representation of plastic relaxation in a (*1*) stressed film via formation of (*2*) misfit dislocations and (*3*) threading dislocations related to them.

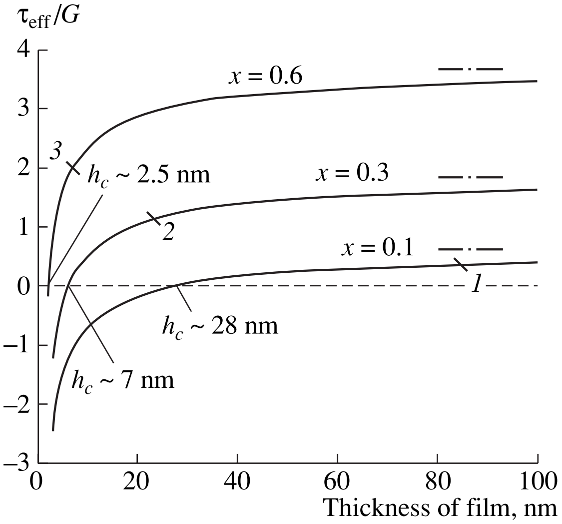


Fig. 2. Calculated normalized effective shear stress as a function of the Ge_xSi_{1-x}/Si(001) film thickness for $x = 0.1$, 0.3, and 0.6. The dash-and-dot lines correspond to the largest values of τ_{eff}/G for $h \longrightarrow \infty$.

formation of a 60° dislocation that can glide in the (111) plane, which is inclined to the interface. The dislocation consists of a segment lying in the interface (the misfit dislocation) and a segment *AB* that emerges at the film surface (the threading dislocation). Plastic relaxation of the film occurs owing to an increase in the length of this MD (segment *BD*) via the motion of a threading segment *CD* in the glide plane. The passage of the dislocation loop through a part of the film reduces plastic strains in this part. Correspondingly, the problem of obtaining perfect and completely relaxed GeSi/Si films can be separated into two subproblems: (I) the attainment of an acceptable rate of film relaxation (reduction of residual elastic strains as the film thickness increases) by introducing MDs and (II) the minimization of the number of threading dislocations. To a certain extent, these two subproblems are contradictory since introduction of MDs occurs via the passage of threading dislocations through the film volume and an increase in the rate of plastic relaxation by increasing the MD density brings about an increase in the density of threading dislocations.

The concept of an effective (excess) shear stress τ_{eff} is used in the studies concerned with the introduction of threading dislocations and their propagation in stressed films (see, for example, [4]); this shear stress governs the processes of MD generation and threading-dislocation propagation in stressed films and is defined by the following expression for a film with thickness *h*:

$$\tau_{\text{eff}} = S\left[\frac{2G(1+\nu)}{(1-\nu)}\right]\varepsilon - \frac{Gb(1-\nu\cos^2\alpha)\cos\phi}{4\pi h(1-\nu)}\left(\ln\frac{\beta h}{b}+1\right). \tag{1}$$

The first term on the right-hand side in formula (1), $[2G(1 + \nu)/(1 - \nu)]\varepsilon$, represents the driving force of plastic relaxation and is equal to the biaxial stress in the film. Here, G and ν are the shear modulus and the Poisson ratio, respectively; and ε is the elastic strain. The quantity $S = \cos\lambda\cos\phi$ is introduced in order to account for the effect of the stress component along the threading-dislocation motion and is referred to as the Schmidt factor. Here, ϕ is the angle between the glide plane and the normal to the interface; and λ is the angle between the Burgers vector b of dislocation and the perpendicular to the line of intersection of the dislocation's glide plane with the interface (this perpendicular lies in the interface plane). The second term on the right-hand side of formula (1) represents the shear-stress component that impedes the propagation of threading dislocations [5]. This component is calculated from the work required to form a unit length of a new MD. In this term, α is an angle between the Burgers vector and the dislocation line. The quantity β is referred to as the dislocation-core parameter and is set (according to recent data) equal to 0.76 for 60° dislocations in a GeSi system [6]. The critical thickness h_c is determined from the equality of τ_{eff} to zero at the initial stage of plastic relaxation, in which case $\varepsilon = f$ (f is the lattice-parameter mismatch); thus, we have

$$h_c = \frac{b(1-\nu\cos^2\alpha)}{8\pi f(1+\nu)\cos\lambda}\left(\ln\frac{\beta h_c}{b}+1\right). \tag{2}$$

This expression was first derived by Matthews and Blakeslee in 1974 [7] on the basis of the balance of forces acting on a threading dislocation. The model [7] referred to as the force balance model is very popular among researchers, and the publication [7] has been cited about 2000 times in scientific literature.

When the film thickness exceeds h_c, the value of τ_{eff} becomes positive; as a result, MDs can now originate and propagate. In Fig. 2, we show the dependences of dimensionless effective shear stress τ_{eff}/G on the Ge_xSi_{1-x} film thickness for $x = 0.1$, 0.3, and 0.6. As the film thickness increases, the dependences tend to the value of $[2(1 + \nu)/(1 - \nu)]\varepsilon$, which is proportional to x. It is well known that, in almost all situations, films grow to thicknesses which greatly exceed the critical thickness corresponding to the origination of the first MDs [3, 8]. For illustration, the points that are marked by numbers and correspond to the film thicknesses equal to $3h_c$ are indicated for each curve in Fig. 2. It can be seen that the effective shear stress increases appreciably as the fraction of Ge in the pseudomorphic film increases, which is bound to affect the rates of MD generation and the propagation of corresponding threading segments.

Houghton [4] suggested the following semiempirical expression for the MD generation rate:

$$\frac{dN(t)}{dt} = N_0\tau_{\text{eff}}^n \exp\left(-\frac{W_n}{kT}\right). \tag{3}$$

Here, N_0 is an adjustable parameter, which [4] characterizes the initial density of the sites for the most probable generation of MDs (this density differs for dissimilar Si substrates); and W_n is the activation energy for MD generation and is equal [4] to about 2.5 eV. On the basis of experimental data [4], the exponent n is equal to 2.5. Thus, comparing the Ge_xSi_{1-x} films with $x = 0.1$ and 0.3, taking into account Fig.2, and using expression (3), we may state that the generation rate of MDs in the films with $x = 0.3$ should be at least an order of magnitude higher than that in the films $x = 0.1$. Correspondingly, the density of threading-dislocation pairs should also be higher.

The final threading-dislocation density depends both on the density of generated MDs and on the velocity of propagation of corresponding threading segments. According to the widely accepted concepts [9] adapted to the threading-dislocation glide in a stressed film [4], the velocity of dislocation motion can be represented as

$$V_d = V_0(\tau_{\text{eff}})^m \exp(-E_\nu/kT), \tag{4}$$

where V_0 is a constant, E_ν is the activation energy for the motion of dislocations by gliding, and the value of m seems to range from unity to two (see, for example, [10]). Consequently, as τ_{eff} increases, the velocity of motion of the MDs' threading branches increases as well. Expression (4) is valid for the initial stage of relaxation. The emerging MD network retards the threading-dislocation motion [6] owing to interaction between local stress fields of dislocations [11].

Under equilibrium conditions and in the absence of barriers, MDs are introduced as long as the thickness of pseudomorphic films exceeds h_c. Stresses in the film are reduced, the critical thickness increases, and MDs are no longer introduced. The film thickness should be increased again in order to introduce a new portion of MDs. Thus, in an ideal situation, the film should plastically relax gradually as its thickness increases. Residual elastic strains can be expressed as

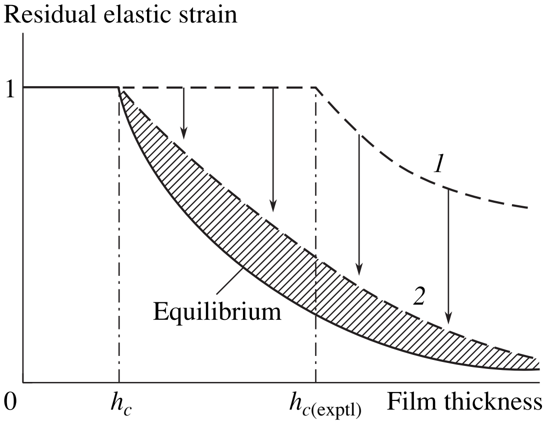


Fig. 3. Schematic illustration of mechanisms governing a decrease in residual elastic strains due to plastic relaxation of the film with an increase in the film thickness. The solid line represents thermodynamic equilibrium in the absence of barriers to the introduction of misfit dislocations; dashed line *1* corresponds to kinetic hindrance to misfit-dislocation generation and to threading-dislocation glide (low growth temperatures), and dashed line *2* represents an experimental quasi-equilibrium dependence (after the prolonged annealing of the heterostructure). Vertical arrows indicate the behavior of relaxation in the course of annealing (the transition from dependence *1* to dependence *2*). Critical thicknesses are also indicated: h_c stands for the thickness calculated according to the Matthews–Blakeslee model [7], and h_c(exptl) denotes the experimental thickness (h_c(exptl) far exceeds h_c if the films are grown at comparatively low temperatures). The hatched lines illustrate the persistent difference between experimental data and the curve calculated for barrierless conditions of introducing misfit dislocations.

$$\varepsilon(t) = f - b_{\text{eff}}\rho(t), \tag{5}$$

where b_{eff} is the component of the Burgers vector along the normal which lies in the interface plane and is perpendicular to the line of intersection of the glide plane with the interface plane, $\rho(t)$ is the linear density of dislocations, and, according to Hu [12],

$$\varepsilon(t) = f\frac{h_c}{h(t)} \quad \text{for} \quad h \ge h_c. \tag{6}$$

In Fig. 3, this dependence of residual elastic strains on the film thickness is shown by the solid line. This equilibrium theoretical dependence corresponds to the largest possible decrease in residual elastic strains as the thickness of GeSi heterostructures increases (based on the highest relaxation rate). As has been mentioned in many publications (see, for example, [3, 4, 8]), the experimentally determined critical thickness exceeds, in the majority of cases, the calculated one (Fig. 3). We may introduce two critical thicknesses: theoretical or equilibrium critical thickness h_c and experimental critical thickness h_c(exptl). A persistent difference between these two critical thicknesses which has been observed

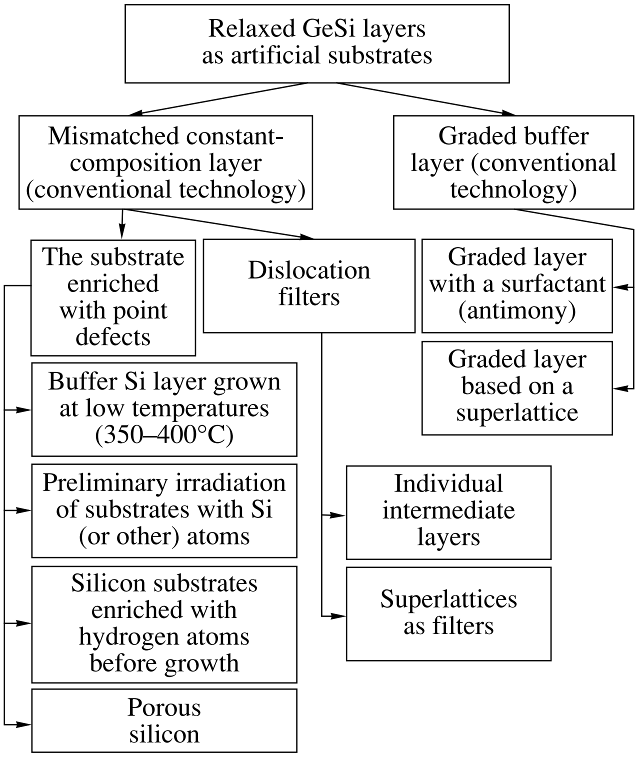


Fig. 4. Classification of the methods for growing plastically relaxed GeSi films, which are conducive to a decrease in the density of threading dislocations in the heterostructure.

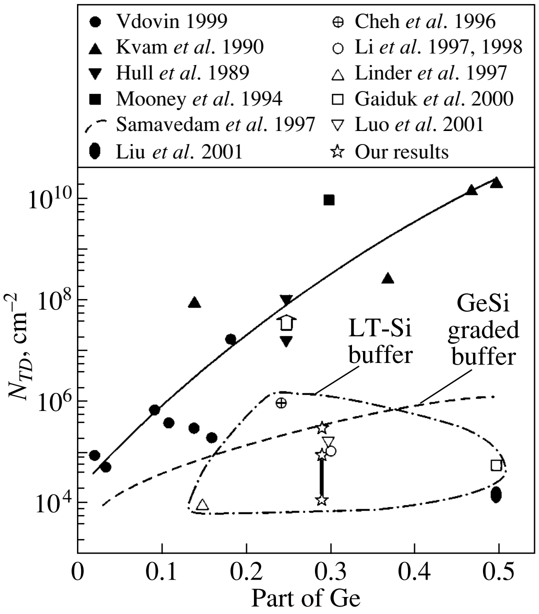


Fig. 5. The density of threading dislocations in Ge_xSi_{1-x}/Si(001) films according to various sources. The solid line approximates the data on the growth of layers with a steplike composition in accordance with conventional technology [16–19] (see text). The dashed line represents the density of threading dislocations in layers using a graded buffer layer [31]. The dash-and-dot line encircles the data on the growth of GeSi layers on an LT-Si buffer [20–22, 24–27, 44]. The filled oval corresponds to a graded Si buffer layer with a surfactant (Sb) [62].

experimentally indicates that various potential barriers play an important role in retarding MD introduction during the growth of semiconductor films. Elevated growth temperatures and postgrowth heat treatments of heterostructures make it possible to approach the equilibrium conditions of MD generation. For example, special studies performed by Houghton *et al.* [13] for Ge_xSi_{1-x} solid solutions with $x = 0.01$–0.15% showed excellent agreement between experimental data and the results of calculations reported by Matthews and Blakeslee [7, 14].

Expression (2) derived for equilibrium conditions defines a certain basic parameter h_c which depends only on the mechanical properties of the specific pair of materials forming the heterostructure, on the degree of mismatch, and on the crystallographic orientation of the interface plane. This parameter is used by researchers as a certain borderline in thicknesses. If the film thickness is smaller than h_c, the pseudomorphic film is thermodynamically stable and MDs are not introduced into it; otherwise, the film is in a metastable state. The onset and rate of plastic relaxation of pseudomorphic films with thicknesses in this range depend on new parameters: on the temperature and duration of the heat treatment of the heterostructure (Fig. 3, dependence *1*) and on characteristics of the films' growth (growth rate, two-dimensional mechanism of growth, role of impurities, and so on). Correspondingly, h_c(exptl) for a specific heterostructure is a drifting quantity which depends on these new parameters. In order to remove (if possible) the restrictions imposed on plastic relaxation of pseudomorphic films, one either has to grow the films at a high temperature [15] or subject the films to postgrowth annealing at elevated temperatures. Nevertheless, as numerous published data indicate (they will be cited in Subsection 2.3), the experimental dependence of the degree of plastic relaxation of a heterostructure on the thickness deviates appreciably from the theoretical (equilibrium) dependence; the former runs systematically above the latter when the aforementioned methods of heterostructure formation are used.

2.2. Comparative Analysis of Various Methods for the Fabrication of Artificial GeSi Substrates

Figure 4 illustrates a classification of the methods for growing GeSi films on Si substrates; these methods are classified according to technical procedures that make it possible to form heterostructures with acceptable structural characteristics. The method involving the growth of films with constant composition is simplest and will be considered first.

The dislocation structure of relaxed films of Ge_xSi_{1-x} solid solutions on Si(001) substrates has been studied in detail for the last 15 years. A typical threading-dislocation density in constant-composition films and its dependence on the Ge fraction x are shown in Fig. 5 based on published data [16–27]. This density is unacceptably high (10^8–10^9 cm^{-2}) for applications in

$Ge_{0.3}Si_{0.7}$ layers. The most widely used temperature for growing such heterostructures is 550°C. We will refer to this variant of growth as the standard. A high density of threading dislocations in these heterostructures is caused by a high density of MDs, each of which is connected to the surface by a pair of "arms" (threading dislocations). According to Hull *et al*. [16], the density of threading dislocations in such a sample is on the order of 10^7 cm^{-2} (correspondingly, the density of generated MDs is on the same level) even at the earliest stages of plastic relaxation, where the degree of this relaxation does not exceed 1%. At the end of the relaxation process, the density of threading dislocations increases to 10^8 cm^{-2} (see the lower and upper inverted filled triangles connected by arrow in Fig. 5).

In order to decrease the threading-dislocation density in a heterostructure, one has to use buffer layers with a varying lattice constant with either a steplike or linear increase in the content of the new component of the solid solution. For more than 30 years, this method was found to be the most appropriate one for growing heterostructures to be used as artificial substrates. Thus, this method is used, for example, to commercially fabricate arrays of light-emitting diodes based on GaAsP/GaAs heterostructures. The basic results of studying these heterostructures were published as far back as the late 1960s [28, 29]. The successful growth of GeSi/Si heterostructures with a gradual variation in the composition of the buffer layer was initiated by Fitzgerald *et al*. [30]. Data on the threading-dislocation density in a graded Ge_xSi_{1-x} buffer layer [31] are shown in Fig. 5. The method for growing relaxed heterostructures with a graded buffer layer yields satisfactory results, since a small composition gradient is chosen (~0.1 Ge fraction per μm); there is only a small elastic strain in the buffer layer at each instant of time. If the parameters of composition variation in the graded buffer layer are chosen properly, the most favorable conditions will be ensured for the generation and propagation of MDs [8, 32, 33]: (i) relatively low stresses in the graded layer (these stresses depend on the gradient steepness) lead to about a low generation rate of MDs; (ii) the MDs are distributed over the entire thickness of the layer with varying composition, which appreciably reduces the effect of blocking a moving threading dislocation by an orthogonally positioned MD; and (iii) a stressed surface region in the growing graded layer gives rise to and continuously supports the driving force for the threading-dislocation glide. In addition to these special features, Shiryaev *et al*. [34] introduce the concept of self-organization for an MD network in a buffer layer with varying composition. It is assumed [34] that it is this factor that is responsible for a low density of threading dislocations at the heterostructure surface, since the ordering of the dislocation network increases the probability of annihilation for threading dislocations.

Unfortunately, the advantages of transition layers with a varying lattice constant gradually become drawbacks as present-day requirements imposed on heterostructures become more and more stringent. Since a small composition gradient is chosen (equal to about 0.1 Ge fraction per μm), then (I) the buffer layers will be thick (1–10 μm), which increases both the growth duration and the consumption of expendable materials (when analyzing the prognosis for the wide use of heterostructures, König [35] noted that a buffer layer with a thickness of about 100 nm would have been ideal from an economical standpoint); (II) the surface roughness, which increases with increasing thickness and can amount to no less than 30–40 nm [36], represents a serious problem in using the layers in modern technology; and (III) the dislocation density of 10^6–10^7 cm^{-2} observed in Ge_xSi_{1-x} solid solutions on Si with $x > 0.5$ is still too high.

2.2.1. Methods based on the modification of the structural properties of Si substrate

Recently, several new methods for forming artificial substrates have been developed; these methods make it possible to significantly improve the results obtained using the standard variant based on fabrication of the buffer layers which have a steplike distribution of composition. First of all, we should mention the use of an Si layer preliminarily grown at low temperatures (LT-Si), which yields good results even if the GeSi films with constant composition are grown on Si substrates [20–24]. At present, this method is best developed among the group of methods (Fig. 4) for which saturation of the substrate with point defects in order to use them as sources of MDs is common. The main methods of this group are represented in the left-hand column in Fig. 4. These methods include preliminary irradiation of the substrate with Si and other ions [37], saturation of the substrate with hydrogen atoms before film growth [38], and use of porous silicon as the substrate material [39]. This group of methods is represented in more detail in Fig. 6 in combination with the characterization of artificial substrates with respect to three main parameters characterizing the structure quality: the relaxation rate, the final degree of smoothness of the heterostructure surface, and the crystal-structure quality. A comparative assessment according to the rate of plastic relaxation is given on the basis of the data reported in cited publications. These data were compared with the results obtained for similar layers grown by the standard steplike method.

Preliminary bombardment of Si substrates with Si ions (method *b* [37] in Fig. 6) is conducive to an increase in the rate of plastic relaxation in GeSi layers; however, this method offers no advantages for the structural quality of corresponding heterostructures over standard steplike growth. Method *c* (see Fig. 6) suggested by Holländer [40, 41] is inconvenient in that hydrogen is implanted into silicon substrate after the growth of the GeSi layer, which should remain pseudomorphic. This layer relaxes plastically only after

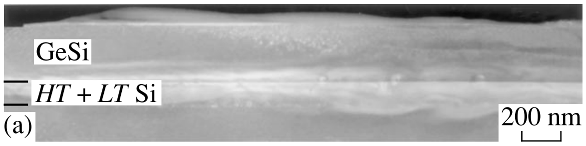
SUBSTRATE WITH SURFACE REGION INTENTIONALLY ENRICHED WITH DEFECTS

Comparison with conventional layers having a steplike composition

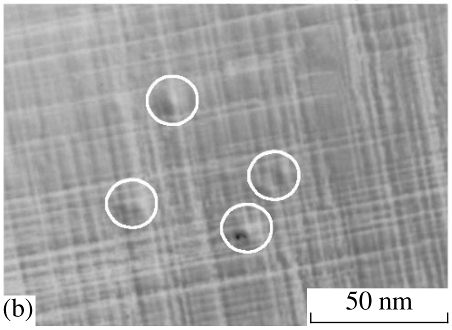
	Plastic-relaxation rate	Smoothness of the layer surface	Standard quality (low threading-dislocation density)
a Epitaxial Si layer grown at low temperatures (300–400°C) H. Chen *et al.* [20] and subsequent publications	–	+	+
b Preliminary bombardment of Si substrate with Si atoms E. Kasper *et al.* [37]	+		–
c Implantation of 25-keV H ions into Si substrate after growth of pseudomorphic GeSi layer with subsequent annealing B. Holländer *et al.* [40]		+	+
d Implantation of hydrogen into Si substrate using low-energy hydrogen plasma (10 eV, before growth) J. Kuchenbecker *et al.* [38]	+	+	+
e Porous Si layer at the Si substrate surface before the growth of a stressed GeSi layer (Our suggestions)			
f An ordered network of screw dislocations after “twist bonding” as a source of misfit dislocations (suggestion) T. Y. Tan, U. Gösele [42]			

Fig. 6. A group of methods based on the preliminary formation of point defects at the substrate boundary and their comparison with conventional methods using three parameters: the rate of plastic relaxation, density of threading dislocations, and surface smoothness.

annealing of the heterostructure. Such a sequence of operations significantly restricts the potential of this method with respect to both layer thickness and composition. Methods *e* and *f* (Fig. 6) rely on the use of substrate composed of either an artificially formed layer of porous silicon or a spacer involving screw dislocations introduced by the method of bonding with misorientation (so-called twist bonding) [42] (this technology will be considered in more detail in Subsection 3.2). However, these methods have not been tested yet.



Cross-sectional TEM image



Etching + Nomarski

Fig. 7. Electron-microscope image of (a) a cross section of a 300-nm-thick $Ge_{0.29}Si_{0.71}$/Si(001) sample with a 50-nm-thick low-temperature silicon (LT Si) underlayer and (b) the sample surface after treatment in the Schimmel etchant. The circles outline the dislocation pits. The cross-sectional TEM image was obtained by A.K. Gutakovskiĭ.

Judging from the characteristics of the comparison given in Fig. 6, methods *a* and *d* involving the use of a buffer layer grown at low temperatures and saturation of the substrate with hydrogen are most promising. However, the latter method has been reported in only a single publication [38] and its further validation and development are required.

The method of growth of a GeSi layer on a preliminarily formed LT-Si buffer layer was reported in [20–24]; in particular, it was shown that completely plastically relaxed 0.5-μm-thick $Ge_{0.3}Si_{0.7}$ films on Si(001) substrates can be obtained with a threading-dislocation density no higher than 10^5 cm^{-2}. Data on the threading-dislocation density in structures with LT-Si underlayers were reported in [20–27] and are outlined in Fig. 5. An appreciable decrease in the threading-dislocation density (even compared with heterostructures based on graded buffer layers) is observed in GeSi/Si structures with an LT-Si underlayer. In addition, the thickness of a heterostructure with an LT-Si layer is much smaller (cf. 0.5 and 3 μm for $x = 0.3$). In Fig. 7a, we show a cross-sectional electron-microscope image of a 300-nm-thick $Ge_{0.29}Si_{0.71}$ sample grown on a 50-nm-thick LT-Si layer. One can see MDs in the interface plane, whereas threading dislocations are not observed. An optical microphotograph of the GeSi layer surface for the same sample after treatment in Schimmel etchant is shown in Fig. 7b [43]. Estimation of the threading-dislocation density on the basis of electron and optical microscopy methods yields 10^4–10^5 cm^{-2}. Since low-temperature molecular-beam epitaxy (MBE) proceeds in significantly nonequilibrium conditions, it is reasonable to assume [21] that the layers grown at a low temperature contain a high concentration of intrinsic point defects, which can represent the main factor conducive to the formation of GeSi with a low density of threading dislocations. Ideas about mechanisms that are conducive to reducing the threading-dislocation density in GeSi films grown on a low-temperature buffer layer are numerous (see Subsection 2.3 for details).

As will be clear from what follows, the main contribution to relaxation in the majority of heterostructures is made by MDs that multiply from a single source. The misfit dislocations, which are closely spaced as a result of the prolonged operation of such a source and have identical Burgers vectors, are largely responsible for the increased roughness of the film surface; this roughness is represented by relatively high hillocks, which act as pinning sites for threading dislocations. According to Fitzgerald *et al*. [31, 32], this mechanism for immobilization of threading dislocations represents one of the main obstacles to the formation of perfect GeSi films based on graded layers. A thick graded buffer layer is necessary to reduce the density of MD sources (see above). At the same time, such a layer ensures plastic relaxation with a small number of secondary sources owing to a high multiplication rate of dislocations; as a result, we have an unacceptable (by today’s standards) roughness of the GeSi layer surface and a relatively high density of threading dislocations. The films grown on an LT-Si buffer layer have less pronounced roughness of the surface [22, 44]. It is assumed that this effect is caused by a more uniform distribution of dislocation sources when an LT-Si buffer is used and, correspondingly, by a lower degree of multiplication of each of these sources.

2.2.2. Dislocation filters

Studies aimed at reducing the density of threading dislocations using so-called dislocation filters, which are represented by layers with different structural characteristics, have a long history [45] and have mostly been restricted to the growth of III–V solid-solution films [46–49] and GaAs/Si heterostructures [50–52]. It is assumed that the filtering properties of separate stressed layers are based on the phenomenon of bending of threading dislocations subjected to tangentially directed forces [45], which is similar to what happens when an MD is formed from a dislocation penetrating from the substrate (see the Matthews model [53]). It would seem reasonable to use a system of stressed layers [a stressed superlattice (SL)] rather than a single stressed layer in order to further reduce the density of threading dislocations. However, the initial explanation for the filtering effect of an SL by the bending of threading dislocations due only to stresses is incomplete and somewhat contradictory in the context of recent data. Indeed, a stressed layer is conducive to bending of threading dislocations; however, it is known that stress-compensated and even unstressed SLs (of the $In_xGa_{1-x}As/In_xAl_{1-x}As$ type) are also efficient dislocation filters [47, 50]. It is assumed [52] that a built-in electric field in an SL with layers which differ appreciably in their electrical parameters is an important parameter of interaction between threading dislocations and the SL. This interaction gives rise to instability of the dislocation segment and is conducive to an increase in the probability of forming a double kink in the dislocation line, thus increasing the velocity of motion of dislocations in the tangential direction.

The use of stressed layers as dislocation filters can be illustrated by the following results. Takano *et al*. [54] grew GaAs films on Si substrates with an $In_xGa_{1-x}As$ intermediate layer (with x as large as 0.15). This layer has a larger lattice parameter than that of GaAs and, as a result, reduces the threading-dislocation density to 10^6 cm^{-2}. Thus, this density decreased by almost two orders of magnitude compared to the situation where there was no intermediate layer. For the same purpose, Sakai *et al*. [55] used a 5-nm-thick Si film introduced into a $Ge_{0.3}Si_{0.7}$ layer on Si(001). Luo *et al*. [56] used an intermediate layer with a thickness of 50 nm. In both cases, a decrease in the threading-dislocation density by about two orders of magnitude was observed.

Unstressed separate layers also act as efficient dislocation filters. For example, Osten and Bugiel [57] grew a $Ge_{0.3}Si_{0.7}$ solid solution on Si(001) using intermediate layers with 10, 15, 20, and 25% of Ge. The density of threading dislocations in the top layer was 10^7 cm^{-2}. After a lattice-matched GeSiC ternary solid solution was inserted into each GeSi solid-solution intermediate layer, the density of threading dislocations decreased to a value lower than 10^5 cm^{-2}. A similar decrease in the density of threading dislocations was observed by Huang *et al*. [58]. In this case, a 100-nm-thick $Ge_{0.2}Si_{0.8}$ solid-solution layer grown on Si(001) at 500°C was inserted into the midsection of a 400-nm-thick layer of the same composition but grown at 750°C. The characteristic features of the last two examples were related to the fact that the so-called insertions had the same lattice parameter as the main layer and, despite the absence of additional bending forces for threading dislocations, acted as dislocation filters. These examples are indicative of a more complex interaction between threading dislocations and additional layers whose properties differ only slightly from those of the main overgrown material.

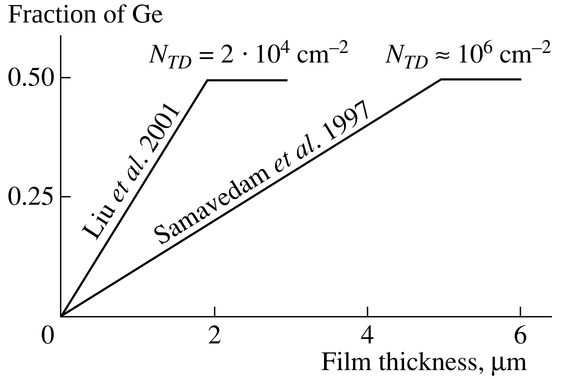


Fig. 8. Linear increase in the Ge fraction in the buffer layer: the data reported by Samavedam *et al.* [31] correspond to conventional technology and those reported by Liu *et al.* [60–62] were obtained using antimony as a surfactant. A schematic representation.

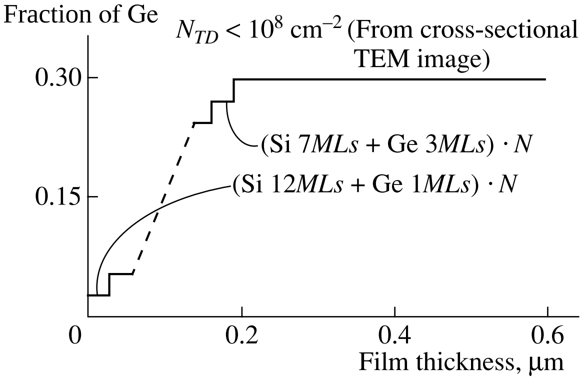


Fig. 9. An illustration of using a buffer layer with a short-period superlattice (according to Obata *et al.* [64]).

2.2.3. Development of gradient methods

As mentioned above, the method of using a graded buffer layer is presently most widely used to obtain artificial substrates. Fitzgerald *et al.* [31, 32, 36, 59] have shown that a comparatively high density of threading dislocations (~10^6 cm^{-2} for $x = 0.3$–0.5 and higher for $x \sim 1$) is attributable to the stoppage (or capture) of moving dislocations by hillocks and depressions on the rough surface. The characteristics of this method can be improved by lowering the roughness of the growth surface. Impressive results were obtained [60–62] by using a monatomic Sb layer, which stabilized the planarity of the growth surface, in addition to using the composition gradient. Antimony is a surfactant, exerts a smoothing effect on the growth surface, and, owing to segregation, remains at the surface during the entire process of growth. Using this method, Liu *et al.* [60–62] managed to appreciably increase the steepness of the gradient in the buffer layer and simultaneously improve the structural characteristics of such artificial substrate. The surface roughness amounted to 2–5 nm (it was 15 nm on the reference-sample surface without using Sb) [61]. In Fig. 8, we show schematically the characteristics of the samples [60–62] compared to those obtained in the standard variant developed by Samavedam [31].

Another method for improving the characteristics of artificial substrates consists in the use of so-called short-period graded SLs [63–66]. Figure 9 illustrates the distribution of the GeSi composition over the depth in this sample [64]. The transition graded layer consists of packs of short-period SLs based on Ge and Si monolayers whose average composition (x) increases as the buffer-layer thickness increases. The fractions of Ge in extreme monolayers are illustrated in Fig. 9. The use of graded SLs makes it possible to reduce appreciably the necessary thickness of the graded layer (in the case under consideration, the reduced thickness is 0.2 μm, as compared with 3 μm in the conventional variant illustrated in Fig. 8), retain or improve the smoothness of the growth surface, and, supposedly, decrease the density of threading dislocations. The attained improvement of these characteristics can be attributed to two factors. It is known that intermediate Si layers in an SL exert a smoothing effect [67–69]. Accordingly, the surface smoothness of artificial substrates with SLs is improved by an order of magnitude compared with conventional structures with a smooth composition gradient (for example, the surface roughness can be reduced by 1–2 nm according to Rahman *et al.* [65, 66]. Further, it is reasonable to assume that the presence of abrupt interfaces between adjacent SL layers, which differ significantly in their composition and lattice parameter, should be conducive to the generation of MDs and, especially, to the propagation of threading segments (see above). Obata *et al.* [64] evaluated the structural perfection of artificial substrates from the absence of threading dislocations in an electron-microscope photograph of a cross section with a length of 1 μm, which sets the detection threshold for threading dislocations at 10^8 cm^{-2}. At the same time, estimations of the threading-dislocation density from images obtained using atomic-force microscopy [66] yield values on the order of 10^5 cm^{-2} or smaller for this density.

Thus, by analyzing modern methods for the formation of artificial substrates, which are based on the plastic relaxation of layers with a differing lattice parameter, we should accept the following three methods as the comparatively developed and most promising. These methods rely on the use of (i) LT-Si buffer layers, (ii) graded layers with Sb as a surfactant, and (iii) graded superlattices; these methods can be combined. For example, Bozzo *et al.* [70] reported the use of a graded GeSi buffer layer terminated by a dislocation filter based on an SL. The threading-dislocation densities in $Ge_{0.25}Si_{0.75}$ layers on Si were reduced to 10^3–10^5 cm^{-2}.

2.3. Possible Mechanisms for the Attainment of a Low Density of Threading Dislocations in Plastically Relaxed Films using GeSi/LT-Si Heterostructures as an example

2.3.1. Relaxation rate and initial density of misfit dislocations

As mentioned above, under the plastic-relaxation rate we mean the rate of decrease in residual elastic strains as the film thickness increases. Figure 10 shows the dependence of the normalized value of residual elastic strain in the $Ge_{0.3}Si_{0.7}$/Si(001) film on the film thickness; this dependence was calculated using the Hu equilibrium model [12] [see expression (6)]. Theoretical dependences based on the generally and widely recognized Gillard–Nix–Freund (GNF) model [6] for $x = 0.35$ are also shown. In the GNF model, a so-called blocking potential of the MD orthogonal network is introduced; the stress field of this potential is calculated taking into account the edge and screw components of 60° MDs. This potential decreases the effective thickness of a growing stressed film and thus decreases the driving force for the propagation of threading dislocations. The hatched area corresponds to the region in which the dependences calculated for four combinations of the Burgers vectors are found. Experimental points are taken from the data reported in [6] and also in other publications [26, 27, 55, 71, 72]. It can be seen that the dependences calculated according to the GNF model are, in general, close to the majority of experimental data; however, these data persistently fall above the results of calculations. Some experimental points deviate appreciably in the direction of either smaller or larger values of residual elastic strain. This is related to special features of growth of specific GeSi films and will be discussed below.

As can be seen from Fig. 10, 100-nm-thick GeSi films grown on an LT-Si buffer layer relax by no more than 15–20% despite prolonged heat treatments at 800–900°C. However, the degree of relaxation increases abruptly as the thickness of the solid-solution film increases. For example, Fig. 11 shows (in the same coordinates as in Fig. 10) two groups of experimental data on the plastic relaxation of $Ge_{0.3}Si_{0.7}$/Si(001) films grown on an LT-Si buffer layer at temperatures of 350°C [26, 27] and 550°C [22, 24]. An abrupt increase in the degree of plastic relaxation in such films is observed even at growth temperatures if the film thickness exceeds 100 nm. Annealing additionally reduces the residual elastic strains in these films.

It is generally accepted that the major part of plastic relaxation of stressed films occurs owing to an increase in the density of MDs due to their multiplication. Beanland [73] draws attention to two waves of plastic relaxation in a stressed layer. The first relaxation wave propagates in the case of a small layer thickness, is caused by primary sources, and, according to different estimations, accounts for 10–20% of complete plastic relaxation. The second wave develops on the basis of sec-

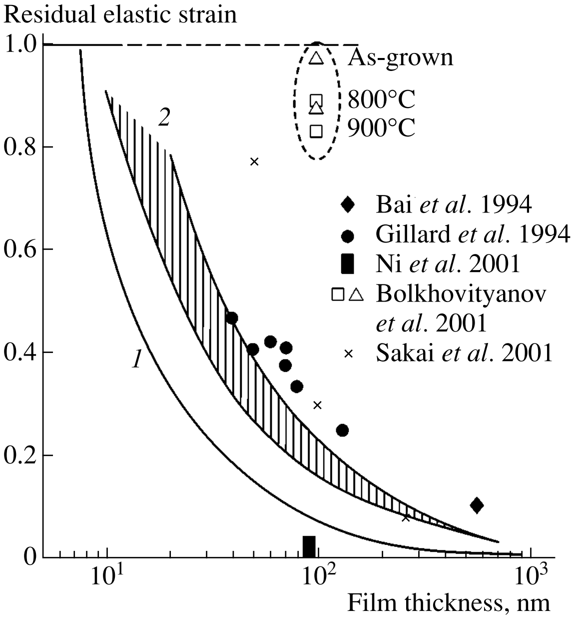


Fig. 10. Normalized residual elastic strains in Ge_xSi_{1-x}/Si(001) films in relation to the film thickness. Comparison of the results of calculations with experimental data. Curve *1* corresponds to the Hu [12] equilibrium model, and hatched area *2* represents a group of dependences calculated by Gillard *et al.* [6]. Experimental points are taken from relevant publications [6, 55, 71, 72]. The dashed oval outlines experimental points that correspond to slowly relaxing Ge_xSi_{1-x}/LT-Si/Si(001) films [26, 27].

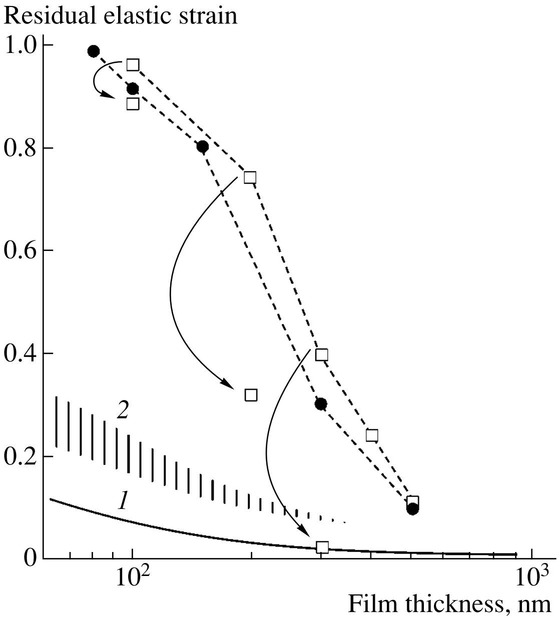


Fig. 11. Normalized residual elastic strains in $Ge_{0.3}Si_{0.7}$/Si(001) films grown on a low-temperature Si buffer layer in relation to the GeSi film thickness. Filled circles correspond to the data reported by Li *et al.* [22, 24]. Squares represent the data obtained by Bolkhovityanov *et al.* [26, 27]. Curved arrows indicate a decrease in residual elastic strains as a result of annealing heterostructures for 1 h at 800°C. Dependences *1* and *2* are part of those shown in Fig. 10.

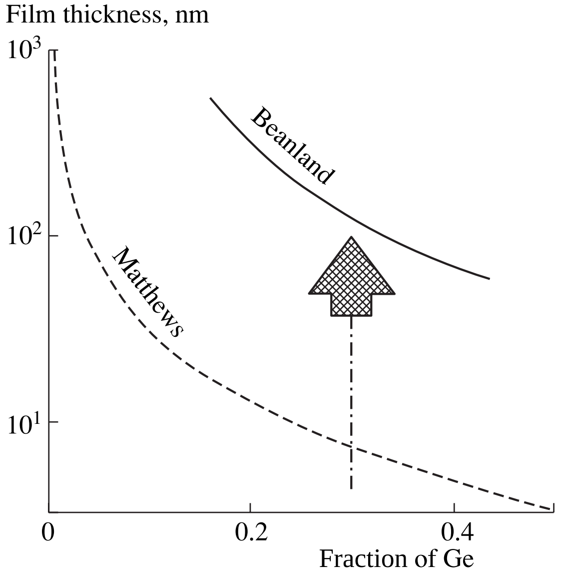


Fig. 12. The critical thickness for the onset of operation of the Frank–Read dislocation source as a function of the GeSi film composition (as calculated by Beanland [73]). Comparison with the conventional dependence of the critical thickness for introducing misfit dislocations on the film composition as derived by Matthews and Blakeslee [7, 14].

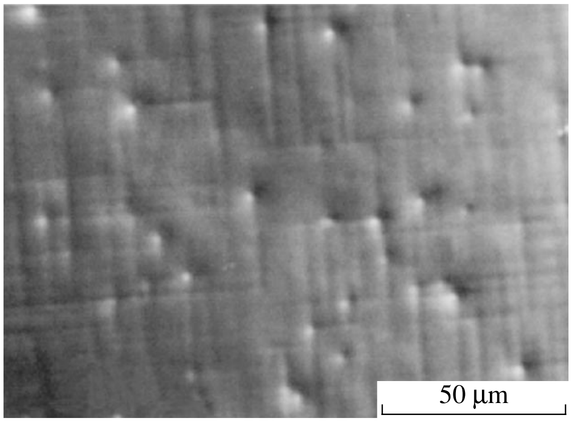


Fig. 13. Threading dislocations (pits) on the $Ge_{0.29}Si_{0.71}$/Si(001) layer surface after treatment in the Schimmel etchant. The GeSi layer thickness is 100 nm; the growth temperature, 350°C; and the degree of plastic relaxation, 5%.

ondary sources related to various variants of the multiplication of dislocations.

According to Beanland [73], the necessary condition for the initiation of secondary sources is that the film thickness exceed the critical one. Figure 12 shows the calculated [73] film thickness for which the Frank–Read source can be effective (and, correspondingly, for which the MD multiplication can occur); this dependence is drawn against the "background" of the curve for the critical thickness of MD introduction [7, 14]. It can be seen that the estimated film thickness corresponding to the onset of MD multiplication is no smaller than 100 nm (the arrow in Fig. 12) for Ge_xSi_{1-x}/Si(001) structures with x close to 0.3. Thus, 100-nm-thick $Ge_{0.3}Si_{0.7}$/LT-Si/Si(001) films, the special features of plastic relaxation of which are illustrated in Fig. 10, have a thickness no larger than that necessary for the actuation of mechanisms of plastic relaxation via the multiplication of MDs; furthermore, the density of primary centers of MD generation is low. Figure 13 shows an optical microphotograph of the surface of a 100-nm-thick $Ge_{0.29}Si_{0.71}$/Si(001) film grown at 350°C [26, 27]. Traces of steps related to MDs and pits corresponding to threading dislocations are observed on the film surface after treatment of the sample in a solution of Schimmel etchant [43]. Taking into account that the degree of plastic relaxation in this film is no greater than 5%, we may assume that the threading-dislocation density of about 10^5 cm^{-2} corresponds to nearly the same density of MDs. This density is two orders of magnitude lower than the threading-dislocation density in GeSi films (triangles connected with the arrow in Fig. 5) grown under standard conditions; in the latter case, the degree of relaxation is no greater than 1% [16]. Consequently, when GeSi films are grown at low temperatures (in the case under consideration, at 300°C), the MD and threading-dislocation density are lower by two orders of magnitude than those in standard films [16]; at the same time, the rate of threading-dislocation glide is higher in the former case since the degree of plastic relaxation is greater. As can be seen from Fig. 11, plastic relaxation of the main portion of elastic strain occurs in thicker films (200 and 300 nm), which can be naturally related to the multiplication of MDs.

It is reasonable to assume that, in order to increase the rate of plastic relaxation in the films to the value exceeding that in conventional films (see dependences *2* in Fig. 10), it is necessary to increase significantly the density of generation sites for MDs. This assumption is validated by the experimental dot (a filled rectangle) shown in Fig. 10 and taken from the publication by Ni *et al.* [71]. Ni *et al.* [71] and Bauer *et al.* [74] showed that the relaxation rate is very high in a GeSi layer grown at a relatively low temperature (150°C) and subjected to subsequent annealing; experimental results reported in the above publications corresponded to nearly 100% relaxation for a 90-nm-thick layer. Apparently, these results are related to the fact that the layer was initially grown at a temperature which was close to the amorphization temperature [71] for the growing layer. Such a layer contains a high concentration of point defects sufficient for the generation of MDs with a high density. At the same time, the threading-dislocation density in such layers, which was determined from analysis of electron-microscope images [74], exceeded 10^{10} cm^{-2}. Thus, an ultrahigh concentration of defects in a GeSi layer is conducive to the formation of MDs with a high density and, correspondingly, to a high rate of plastic relaxation. However, as a result, one obtains a high density of threading dislocations.

We may assume that optimal growth conditions should exist for the formation of relaxed GeSi films with a low density of threading dislocations. For example, Luo *et al.* [44] showed that an LT-Si buffer layer grown at 400°C is most appropriate for subsequent epitaxy of GeSi layers with a low density of threading dislocations. Studies based on electron–positron annihilation spectroscopy [75–77] showed that the layers grown using the low-temperature (200–400°C) epitaxy of silicon and its solid solutions with germanium contain a high concentration of vacancy-type defects (~10^{17}–10^{18} cm^{-3}). According to Ueno *et al.* [77], the largest vacancy cluster (containing more than ten vacancies) was observed in an Si layer grown at 400°C. It is at this temperature that the discoverers of this method (Chen *et al.* [20]) for obtaining GeSi films with a low threading-dislocation density grew the LT-Si buffer layer.

2.3.2. The rate of motion of threading dislocations

The magnitude of residual elastic strains should be approximately the same in the layers with a high density of "short" MD segments and in the layers with a low density of extended MDs. However, it is evident that the threading-dislocation density is bound to be higher in the former case. Consequently, it is preferable to combine a low MD generation rate with a high propagation velocity for threading dislocations. Thus, it is necessary to be able to control both processes separately. It is worth noting that, in the majority of studies concerned with a discussion of mechanisms which are conducive to the formation of heterostructures with a lowered threading-dislocation density, attention was primarily focused on the assumption that annihilation of threading dislocations is enhanced; the possibility of increasing the glide rate of these dislocations was not considered at all. It is reasonable to assume that the presence of a high concentration of vacancy-type defects [77], which diffuse from the LT-Si layer and accumulate in the vicinity of MDs, can decrease the dislocation-core energy [78] in a structure with an LT-Si underlayer. Additional arguments can be found in the publication by Fedina *et al.* [79], where it was shown experimentally that, under conditions of a high concentration of point defects, microregions with an absence of dangling bonds were formed, whereas the defect-displacement vector decreased. As a result, the linear tension of an MD extended section [i.e., the right-hand side of expression (1)] decreases; correspondingly, the propagation velocity of threading dislocations increases. The data on the increase (by two orders of magnitude) in the rate of motion of dislocations in silicon saturated with hydrogen can serve as indirect evidence in support of the above mechanism [80].

Additional confirmation of the fact that this mechanism is feasible can be obtained by paying attention again to the experimental point (filled rectangle in Fig. 10) reported by Ni *et al.* [71]. As can be seen from Fig. 10, this experimental point lies significantly lower than the relevant dependence for equilibrium critical values of thickness calculated according to the Hu model [12]; i.e., this point lies in the region where a 100% degree of relaxation is energetically unfavorable. If the data reported in [71, 74] are reliable, this inconsistency between experiment and the dependence calculated according to the Hu model [12] can be attributed to a significant decrease in the work needed for the formation of a new MD of unit length [the right-hand side of expression (1)]. In these conditions, according to expression (1), critical values of thickness for the introduction of MDs become smaller than those in conventionally grown GeSi layers. In addition, a new calculated dependence for critical thicknesses is bound to run below the standard one shown in Fig. 10.

The aforementioned assumptions relate an increase in the motion rate of threading dislocations to variation in the effective shear stress τ_{eff} in expression (4). Another possibility can be also considered. A variation in the glide velocity of dislocations can also be related to variation in the activation energy of this process. As is well known, the widely accepted model of dislocation motion is the model based on the formation of double [81] and single kinks in dislocations. Due to thermal fluctuations or the effect of stresses, a double kink (DK) can originate in the dislocation line. After attaining a critical size, the DK dissociates into two single kinks, which propagate in different directions; this ultimately results in the transition of the dislocation line to a neighboring valley of the energy profile. Thus, the rate of glide of dislocation is controlled by the kink-formation energy F_k and the height of the energy barrier for the migration of the kink W_m. The activation energy E_v of dislocation motion in expression (4) consists of two components: the activation energy for formation of a double kink and the activation energy for kink migration, i.e., $E_v = 2F_k + W_m$. Measurements of the motion rate for dislocations in stressed structures were used to reveal that the activation energies for the motion of 60° dislocations E_v are equal to about 2.2 eV for Si and GeSi [4, 16, 82, 83]. These activation energies are much lower in GaAs: 0.89–1.3 eV for α dislocations and 1.24–1.57 eV for β dislocations [82]. In our opinion, these data for GaAs were the main reasons why good results were achieved earlier in producing high-quality artificial substrates made of III–V compounds and were more dependable than in the case of GeSi. Gottschalk *et al.* [84] summarized experimental data on F_k and W_m in Si: $W_m = 1.2$–1.8 eV and $F_k = 0.4$–0.7 eV.

These energies were measured and calculated for Si and GaAs in the conventional crystalline state. However, they may decrease if the growing layer contains a high concentration of point defects. Correspondingly, the rate of motion of threading dislocations may increase. For example, Öberg *et al.* [82] noted that, according to both experimental data and the results of

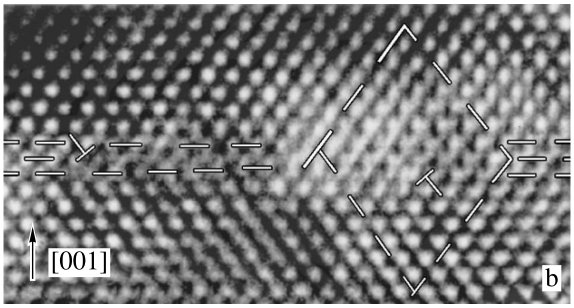


Fig. 14. An HREM image of a dislocation dipole in the (001) plane. A Burgers contour encloses the right-hand core of the dislocation dipole. The initial mismatch amounts to 0.9%. The photograph was made available to us by L. Fedina (reproduced with permission of the authors [88]).

calculations, the activation energy for the motion of dislocations is lower in doped silicon. Yamashita *et al.* [80] reported that the activation energy for the glide of dislocations decreased from 2.2 to 1.2 eV and the rate of their motion increased by two orders of magnitude after silicon was enriched with atomic hydrogen. Therefore, a decrease in both F_k and W_m under the effect of a high concentration of point defects can be considered a reasonable assumption. It is noteworthy that a thin layer inserted into the main film and having a different composition [54–57] or a spacer grown at low temperatures [58] can play the same role as defects; i.e., these layers can increase the probability of the formation of a double kink in the dislocation line and can thus increase the rate of motion of threading dislocations. It was also observed [54–57, 58] that the threading-dislocation density is lower in films with inserted foreign layers than in films without these layers.

2.3.3. Improvement of conditions for the annihilation of threading dislocations

The rate of annihilation of threading dislocations can increase owing to an increase in the radius of interaction between threading dislocations that move in closely spaced glide planes; this effect can also be related to a high concentration of point defects [37]. Typically, stressed layers are grown at temperatures such that the climb of dislocations can be ignored. A high concentration of point defects formed as a result of either irradiation or growth of a low-temperature buffer layer increases the probability of the inclusion of this mechanism for the climb of dislocations in the process of annihilation of threading dislocations which propagate in closely spaced glide planes. An assumption about the origination of an ordered network of threading dislocations at the initial stage of plastic relaxation also relies on the emergence of additional conditions which are conducive to the annihilation of threading dislocations [25, 41]. Trinkaus *et al.* [41] assume that there is a certain ordering of threading dislocations as a result of their generation at microvoids formed after implantation of hydrogen into a preliminarily grown and initially pseudomorphic GeSi layer, whereas Gaiduk *et al.* [25] and then Bolkhovityanov *et al.* [26, 27] suggested a more elegant model; the latter will be considered in detail in the next subsection.

2.3.4. An ordered network of threading dislocations

It is assumed that a silicon underlayer grown at low temperatures and enriched with point defects can serve as a source for the origination and development of an ordered misfit-dislocation network. The significance of ordering lies in the fact that this network should be formed of single-type dislocations; reactions between these dislocations should be energetically favorable and lead to the annihilation of threading dislocations. The issue concerning the properties of the sources required for the generation of misfit dislocations is most important in this context.

It is reasonable to assume that, as the density of primary heterogeneous MD-generation sources related to various inhomogeneities in the substrate surface decreases, the main sources of MD generation become associations of intrinsic defects at the heterostructure interface. The number and atomic structure of these associations are governed by the conditions of low-temperature growth of the Si buffer layer and by the properties of the adjacent portion of a stressed GeSi layer (or by the structural state of Si substrate after irradiation). It is known [85, 86] that annealing of silicon containing a high concentration of point defects gives rise to specific rodlike defects in {311} planes. These defects are oriented along the ⟨110⟩ directions and are composed of interstitial atoms located in the {311} planes in the form of a hexagonal Si monolayer. Under certain conditions, the rodlike defects become the sources of dislocation loops [87]. The formation first of vacancies in the plane parallel to the interface and then of dipoles of 60° dislocations was observed after direct irradiation of pseudomorphic GeSi/Si(001) layers with electrons in a high-resolution electron microscope (HREM) (Fig. 14) [88].

Heterogeneous sources of dislocations at the substrate surface are formed before the onset of growth of the stressed layer and exist irrespective of the presence of this layer. These sources are activated both when the temperature is elevated and when the thickness of the pseudomorphic layer is increased beyond the critical thickness; as a result, it is generally assumed that a complete set of dislocations is formed in the relaxing film. Clusters composed of point defects are initially absent in the LT-Si (or (LT-GeSi) layers and appear only under certain conditions, in particular, when there is a field of internal stresses in the course of growing the stressed layer. We may assume that the diversity of the crystallographic shapes of these clusters becomes limited when they are formed in the presence of a biaxial stress field. Under conditions of a plane-stressed state of the heterosystem, the clusters become ordered with respect to both the crystallographic orientation and spatial distribution. As a result, the formed clusters have a specific crystallographic orientation and are conducive to the generation of a more limited variety of MDs; in other words, as Gaiduk *et al.* note [25], "a self-assembled network of primary dislocations is formed." In this case, the annihilation rate of threading dislocations is bound to increase drastically compared to the conventional case (a decrease in the density of threading dislocations is inversely proportional to the film thickness [89]), which ultimately brings about a lower density of threading dislocations.

Thus, under the effect of self-organization of the primary MD network we mean the following sequence of events: point defects, which are present in the LT-Si and (or) LT-GeSi layers, are grouped into clusters in the vicinity of the interface during the growth of the pseudomorphic GeSi layer; the 60° MDs are then generated on the basis of these clusters. The determining factor of this process is the fact that the above structural rearrangements occur under the effect of a stress field of the growing pseudomorphic solid-solution layer. Despite the apparent consistency of the model, which implies ordering of MDs at the initial stage of formation of the dislocation network and, as a consequence, an increase in the probability of threading-dislocation annihilation, direct observations indicating that this mechanism is plausible are lacking in the available publications.

2.4. Basic Methods for the Fabrication of Artificial Substrates Based on Plastic Relaxation of Heterostructures

Thus, after more than 20 years of attempts to grow perfect GeSi/Si heterostructures with constant-composition films, the crystalline quality of these structures leaves much to be desired. This manifests itself in a high threading-dislocation density, which increases with an increasing Ge fraction (see the solid line in Fig. 5). As the mismatch between the lattice parameters of the film and substrate becomes more significant, the glide rate for threading dislocations increases; however, the number of these dislocations increases as well. In our opinion, the observed high density of threading dislocations is governed by the relation between the density of generated MDs and the velocities of propagation of threading segments in GeSi heterostructures grown under similar conditions (standard Si substrates and conventional growth conditions of GeSi films); the terms of the above relation have common driving forces, and the relation itself varies within a narrow range.

Recently, new methods for treating substrates have been developed and new conditions of film growth have been suggested; these innovations made it possible to affect the above processes independently, which resulted in the improvement of the crystalline quality of grown GeSi films. For example, the density of the centers for the heterogeneous generation of MDs can be reduced significantly by thorough preepitaxial treatment of the substrate surface and by overgrowth of the Si buffer layer (with a thickness of 50–100 nm); this layer moves the GeSi/Si interface away from the substrate surface. As follows from the above discussion, the rate of the threading-dislocation propagation can be increased by a number of methods. These methods include introducing point defects into the substrate and the interfacial region of the heterostructure and the formation of "insertions" within the heterostructure in the form of separate layers or superlattices. The efficiency of these methods in increasing the rate of threading-dislocation glide has been observed so far only in experiments in which the Si substrate is enriched with hydrogen atoms [80]. In other cases, the effect of these methods is within reasonable assumptions based on the analysis of experimental data related to efforts to improve the structural properties of the heterostructure.

The data listed in Table 1 make it possible to correlate the new methods with possible mechanisms for reducing the threading-dislocation density, which were discussed above. It can be seen that, in the majority of cases, explaining the positive effect of a certain factor will be tentative. Thus, these new methods require more thorough experimental studies with the aim of gaining insight into specific mechanisms that bring about an improvement in the structural properties of relaxed GeSi films.

Nevertheless, if we combine the analysis of the aforementioned experimental data with basic concepts of the theory of plastic relaxation in heteroepitaxial films, we can envisage the following methods that are conducive to a decrease in the density of threading dislocations in relaxed films and to an acceptable morphological quality of these films:

(I) The MD density caused by the activation of primary centers of MD generation should be low (~10^4–10^5 cm^{-2}), which is ensured by thorough preepitaxial treatment of the substrate surface, absence of contaminants during growth, and overgrowth of an Si buffer layer.

(II) It is necessary to satisfy the conditions for the activation of threading-dislocation motion and for an increase (or retention at the same level) of the propagation of these dislocations. Suggested methods consist in introducing a high concentration of point defects and forming additional inhomogeneities in growing films by introducing separate layers with a different composition or superlattices.

(III) It necessary to provide conditions for an increase in the probability of annihilation of threading dislocations (presumably, a high concentration of point defects and ordering of the dislocation network can be conducive in this respect).

(IV) Special attention should be paid to ensuring a two-dimensional mechanism of growth and planarity of the growth surface. These requirements can be met by

Table 1. The factors that are conducive to decreasing the density of threading dislocations in relaxed layers with lattice-parameter mismatch and realization of these factors in various methods

Method	Factor						
	a decrease in the density of primary misfit dislocations	an increase in the propagation rate of threading dislocations	promotion of threading-dislocation annihilation	an ordered misfit-dislocation network conducive to threading-dislocation annihilation	a decrease in the capture of threading dislocations by a rough surface	a decrease in the immobilization of threading dislocations by misfit dislocations	number of publications
1. Graded buffer (conventional technology)	Experiment and theory [8, 32, 33]	Constant rate expected on the basis of the model [33]		Assumption [34]		Expected on the basis of the model [33]	>10
2. Graded buffer with Sb as a surfactant	Expected on the basis of the model [33]	Constant rate expected on the basis of the model [33]			Reduction of roughness, experiment [61]	Expected on the basis of the model [33]	3
3. Graded buffer based on short-period superlattices	Expected on the basis of the model [33]	Should be expected on the basis of assumptions [52]			Circumstantial evidence, this review	Possible, since misfit dislocations reside in different planes	4
4. Filters based on superlattices		Assumption [52]	Assumption [8, 52]				2
5. Individual inserted layers		Assumption, this review	Assumption [45]		Assumption [55]		4
6. Buffer layer grown at a low temperature	Experiment [26, 27]	Assumption based on circumstantial evidence [79], this review	Assumption [37]	Assumption [25–27]	Assumption [22, 24]		>10
7. Enrichment of silicon substrate with hydrogen		Experiment [80]					2
8. Implantation of hydrogen under the pseudomorphic GeSi layer with subsequent annealing				Assumption [41]			3

inserting thin layers of either a pure Si layer or short-period (graded) SLs into the film or by using antimony as a surfactant.

The conditions of growth of heterostructures intended for use as artificial substrates should be chosen on the basis of the aforementioned special features.

3. "COMPLIANT" AND "SOFT" SUBSTRATES: EXPECTATIONS AND REALITY

3.1. Basic Concepts

The idea of using a compliant substrate is based on the effect related to redistribution of elastic strains between the pseudomorphic layer and the substrate if the thickness of the latter is comparable to the thickness of the growing layer (see, for example, the monograph [90]). In Fig. 15, we show the schematic representation of a structure in which this effect can be used. It is assumed that a thin membrane, which serves as a compliant substrate, can move freely in the lateral direction without, however, losing contact with the thick supporting substrate. Strains in the pseudomorphic layer, with allowance made for the substrate thickness, can be written as [90]

$$\varepsilon_f = \frac{d_0}{d_0 + h}\varepsilon_0, \qquad (7)$$

where d_0 and h are the thicknesses of the compliant substrate and the layer, respectively; and ε_0 is the total elastic strain in the case of a thick substrate. The smaller the thickness of the substrate–membrane, the smaller the total strain in the layer.

The term "compliant substrate" was introduced into scientific literature by Lo [91]. It was assumed that, under certain conditions (for example, a small thickness of the membrane), the elastic strain in a growing pseudomorphic film decreases as the film thickness increases. In this case, the introduction of MDs into the films becomes energetically unfavorable at any film thickness; correspondingly, the process of plastic relaxation of stresses in the growing film may not set in at all. Since the idea of using a compliant substrate was quite clear and promised real advantage in improving the crystalline quality of growing films with a differing lattice parameter, it was rapidly accepted by the scientific community; specifically, experiments with various materials were conducted [92–104], theoretical calculations of the critical thickness and relaxation of stressed films [105–109] were performed, and the relevant reviews were published [3, 110–114].

3.2. Technical Realization

To date, two variants of fabricating compliant substrates have become known and implemented.

(I) The first variant relies on the use of silicon-on-insulator (SOI) substrates [94, 95]. In these structures, a silicon layer on oxide is thinned and becomes a thin membrane (substrate) for the growth of the heteroepitaxial film, whereas the oxide layer is treated as a viscous spacer, which ensures sliding of the heterostructure with respect to the main substrate. In addition, other methods for the formation of an amorphous viscous spacer between the main substrate and the membrane have been used. These methods include (i) the implantation of B into the SiO_2 layer in order to reduce its viscosity [98] and (ii) the bonding of the GeSi/Si heterostructure to the Si substrate using a SiO_2 intermediate layer [100]. Recently, Luo *et al.* [99] reported the use of a compliant substrate with an underlayer of borosilicate glass for the growth of a Ge_xSi_{1-x} solid-solution film with $x = 0.25$. This underlayer was formed by ion implantation of B and O into the buried SiO_2 layer. With respect to the threading-dislocation density in GeSi films, the result reported in [99] was comparable to the best data obtained in other studies using thick graded buffer layers or silicon buffer layers grown at low temperatures.

In a version of this method used for III–V compounds, a GaAs/AlGaAs/GaAs heterostructure is bonded via an intermediate layer (which will play the role of a "soft" substrate in what follows) to the supporting substrate [93, 96, 97]. The heterostructure substrate and the AlGaAs layer are then dissolved in different etchants [AlGaAs is used as a stopper layer in etching the GaAs substrate according to the well-known technology for the fabrication of photocathodes (see, for example, [115])]. The remaining GaAs film on the "soft" underlayer is treated as a compliant membrane in the course of growing stressed InGaAs films.

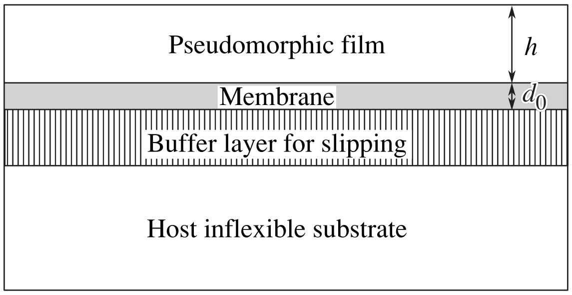


Fig. 15. A schematic heterostructure model including a thin membrane which can slide over the supporting substrate.

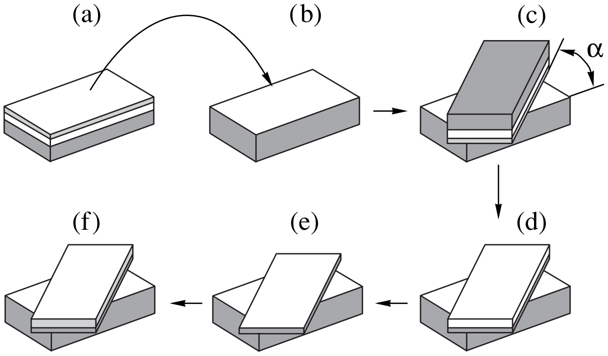


Fig. 16. Schematic representation of the formation of a compliant substrate according to the twist-bonding technology: (a) a preliminarily grown GaAs/AlGaAs/GaAs heterostructure, (b) a supporting GaAs substrate, (c) bonding of a and b by welding with rotation by an angle α, (d) etching off of the GaAs substrate, (e) etching off of the stopping AlGaAs layer (the compliant-substrate structure is finally formed), and (f) an InGaAs layer is grown on the compliant substrate.

(II) The second variant consists in bonding with misorientation (the so-called twist bonding) [42, 101–104]. In this case, the GaAs/AlGaAs/GaAs heterostructure is bonded directly to the GaAs substrate (without intermediate layers), with the crystallographic orientations of the components of the bonded pair being different. In the ideal case, twist boundaries with a weakened bond structure and an ordered network of screw dislocations are formed between joined wafers. Eventually (as illustrated in Fig. 16), the GaAs substrate and the AlGaAs stopper layer are etched off in the same way as in the previous variant. It is assumed that, in the course of subsequent growth of a stressed layer on a thin GaAs layer, the latter is compliant since the region containing screw dislocations is conducive to the sliding of the GaAs layer over the supporting substrate [101]. Ejeckam *et al.* [101] reported on the efficiency of using such a substrate in their pioneering studies concerned with the heteroepitaxy of InSb on GaAs. In this case, the lattice-parameter mismatch amounts to 14.7%. According to Ejeckam *et al.* [101], it is possible to reduce the density of threading dislocations to 10^6 cm^{-2}.

It is noteworthy that both methods are based on bonding technology, which is sophisticated and costly. It seems that the method based on the use of a viscous amorphous layer, which is formed “automatically” during the growth of crystalline strontium titanium oxide, is more promising [116]. The authors of the latter publication, in attempting to improve quality of a GaAs/Si structure, introduced an additional $SrTiO_3$ layer between the Si substrate and GaAs film. This layer has a lattice parameter which is intermediate between those of Si and GaAs; this circumstance is conducive to a more gradual (two-stage) transition from Si to GaAs. In addition, it has been found [116] that oxygen diffusing from $SrTiO_3$ into the Si substrate forms a SiO_x amorphous spacer in the substrate; it is believed [116] that this spacer gives rise to the effect of compliance. This method was used to grow GaAs layers on Si substrates that were 12 inches in diameter; the authors state that the properties of these layers were no different from those of homoepitaxial GaAs.

3.3. Mechanisms of Relaxation

It has been demonstrated repeatedly that the structural quality of relaxed films grown on compliant substrates is indeed higher than in the case of films grown otherwise; the relevant results are summarized in published reviews [112–114]. However, the relaxation mechanism based on redistribution of elastic strains between the film and elastic membrane (or a region with decreased elastic constants, e.g., a region of porous silicon) cannot be dominant, even though this mechanism is suggested in the majority of publications. In fact, if the film on the substrate initially grows pseudomorphically and then relaxes elastically without the formation of MDs, the strain in this film is transferred to the compliant membrane. The final lateral size of the film after elastic relaxation should be larger than the initial size (larger by the magnitude of mismatch). Consequently, if the substrate size is reasonable, both the epitaxial film and the membrane should slide unimpeded over the inflexible substrate by large distances (by fractions of a millimeter, or by several millimeters in the case of 12-in. wafers). Despite a large body of experimental data and the analysis of it in relevant publications, sliding of an extended relaxing film over the substrate was not detected.

Typically, the interface between the membrane and substrate involves a number of various defects (steps, inclusions, impurities, and so on), which hinders the free sliding of a membrane by large distances and makes this slide impossible without detachment of the heterosystem from the inflexible substrate. The same problem also persists in the case of plastic relaxation of the membrane if the processes of introduction, glide, and interaction of dislocation half-loops are confined to the compliant (“soft”) intermediate layer. The process of slide of the layer–membrane pair over the inflexible substrate should set in at different (random) sites of the substrate surface, which must inevitably result in the counterslide of separate regions and the formation of a cellular structure. In addition, the regions of perfect material are expected to alternate with folds, cracks, or highly imperfect zones.

It has been shown recently [117, 118] that relaxation of stressed films on a viscous substrate occurs via elastic extension of the film due to the film’s slide over the above spacer only if the latter has a small lateral size. For example, Yin *et al.* [117], when studying the characteristics of relaxation of 30-nm-thick pseudomorphic $Ge_{0.3}Si_{0.7}$ islands connected to the Si substrate via a layer of borosilicate glass, found that the mesa islands relax in the course of annealing; this relaxation is mainly due to buckling. Relaxation of elastic strains in these islands as a result of slide of the film over the interface has been observed to prevail over buckling only at the corners of the islands with diameters ranging from 10 to 20 μm. Tezuka *et al.* [118] showed that GeSi mesa islands which were 5 μm or less in diameter and had been grown on SOI substrates relaxed completely without the formation of MDs as a result of annealing at 1000–1200°C. This is evidenced by the absence of so-called cross hatches, which are markings of dislocations’ outcrop. However, extended regions (with sizes of 300 μm or larger) of GeSi films on the same substrate contain surface cross hatches, which constitutes direct evidence that these layers are plastically relaxed.

The use of continuous intermediate porous buffer layers, which are expected to act as “lubricants”, is inefficient in the context of the conventional interpretation of the phenomenon of compliance. Since the porous layer is rigidly linked to the main Si substrate, such a layer cannot freely slide over the supporting substrate. The porous layer has low mechanical strength and is more likely to be used as a plastically relaxing membrane. The forming of small-sized mesa regions made of porous silicon and covered with a thin silicon membrane seems to be the most appropriate method for realizing the idea of a compliant substrate [119]. These mesa regions have a small Young’s modulus (at least an order magnitude smaller than the Young’s modulus of solid silicon [120]) and can accommodate strains in the heterosystem; in addition, the small sizes of these regions make elastic relaxation possible due to distortion of the crystal lattice of porous silicon, since the variation in the absolute dimensions of the film does not exceed fractions of a micrometer. Corresponding calculations were carried out by Novikov *et al.* [119]. Figure 17 illustrates the effect of the width of a porous mesa strip (L = 5, 10, and 30 μm) with a thickness h_{mesa} = 1 μm on the degree of elastic relaxation in a $Ge_{0.3}Si_{0.7}$ layer. It can be seen that the layer grown on 30-μm-wide porous Si mesa strip ($h_{mesa}/L \sim 0.03$) is virtually unsusceptible to elastic relaxation. The "softness" of the mesa strip is caused by its porosity and begins to manifest itself only when the transverse size of the mesa-strip decreases and its height increases, i.e., when the ratio h_{mesa}/L (the aspect ratio) increases.

Thus, the mechanism of elastic relaxation in a stressed film due to the sliding of this film over a viscous substrate can be efficient only at small distances in the mesoscopic range, i.e., in the situation where the film is of the island type owing either to its formation (so-called quantum dots [121]) or if it was grown on intentionally formed mesa islands.

On the basis of the above discussion, we should consider the mechanisms of plastic relaxation in films grown on "compliant" substrates. The main contribution to a reconsideration of relaxation mechanisms in such films was made by Kästner and Gösele [113]. They returned again to plastic relaxation of strains as an alternative to elastic relaxation and suggested a modified concept of plastic relaxation; this concept consists in the following. The conventional variant of formation of MDs at the interface between a stressed film and a substrate–membrane is illustrated in Fig. 18a. If there is an amorphous or amorphized spacer near the interface, an MD sinks in this spacer (Fig. 18b); this phenomenon is caused by the fact that an MD is pulled from the film–membrane interface by forces which are similar to image forces acting on the dislocation line near the film surface. As in the case of a free surface, a dislocation leaves a step at the interface between the membrane and the "lubricating" layer (see dashed lines in Fig. 18). The additional energy caused by the origination of such a step is much lower than the MD energy at the interface (similarly to what happens in the case of a free surface). The difference between the above two energies represents the driving force for the displacement of an MD to the interface between the membrane and "lubricating" layer. Correspondingly, the work spent on the MD formation decreases.

Since the retarding forces inhibiting the propagation of threading dislocations decrease [see expression (1)], the critical thickness for the introduction of MDs decreases rather than increases, as follows from calculations based on the model of redistribution of elastic strains between the film and a compliant membrane. In this case, the velocity of motion of threading dislocations increases, which contributes to a decrease in the density of these dislocations. A similar situation is possible if porous silicon or a system of screw dislocations after the twist-bonding procedure are used as "lubricating" layers. Experimental verification of these two cases is lacking at present; therefore, these methods are listed as suggestions. In the latter case, a periodic network of strains in the vicinity of the interface between the stressed film and the membrane can serve [42, 111] as the site of origination for an ordered network of MDs, which is conducive to the annihilation of threading dislocations.

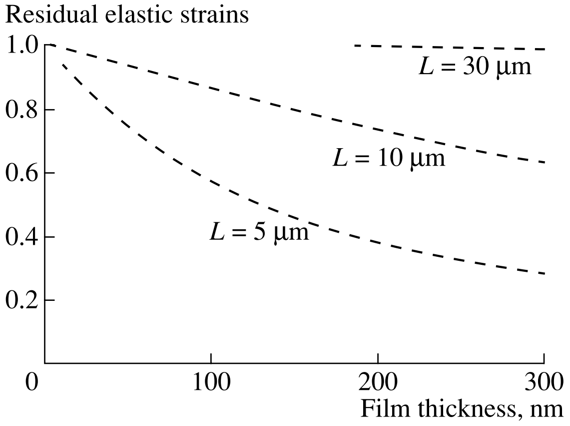


Fig. 17. The behavior of elastic relaxation of strains in GeSi film grown on a porous silicon strip with a thickness of 1 μm and a width L as a function of the film thickness [119].

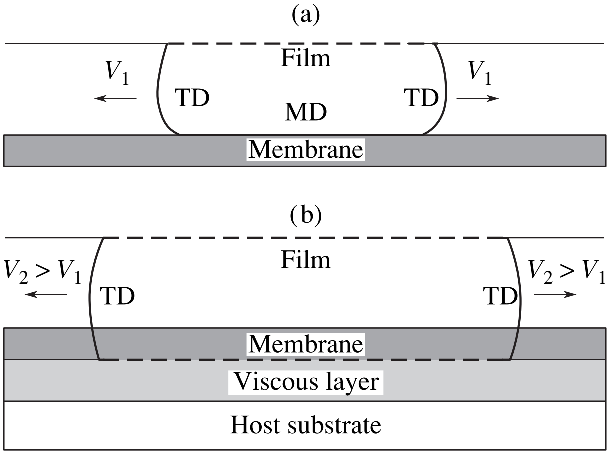


Fig. 18. "Disappearance" of a misfit dislocation in a heterostructure grown on the substrate–membrane, which is positioned on a viscous amorphous spacer (according to Kuastner and Gösele [113]). TD stands for threading dislocation; and MD, for misfit dislocation.

Recently, Pei *et al.* [122] also suggested the idea of "pulling" MDs from the interface between the stressed film and Si membrane to the interface between the Si membrane and SiO_2. By growing GaAs on SOI substrates with thinned Si membranes 100 and 200 nm thick, it was possible to attain the smallest half-width of the X-ray rocking curve (128″) for GaAs films grown on Si [122].

Thus, we return again to the concept of modifying the plastic-relaxation mechanism; this concept was outlined above in Subsection 2.4 and consists in the following. In heterosystems with intermediate layers (grown at low temperatures or subjected to ion bombardment) including viscous spacers, the velocity of propagation of threading dislocations increases. As a result, the relation (between the generation rate of MDs and the velocity of propagation of threading disloca-

Table 2. The basic characteristics of SiGe/Si heterostructure bipolar transistors

Manufacturer	Transit-time frequency for the base, f_T (GHz)	Maximum frequency of oscillation, $f_{\max}$ (GHz)	Design parameter of complementary MOS transistors (μm)
AMSINT	35	30	0.8
AMTEL	30, 50	50, 50	0.35
AMTEL	30, 50, 80	30, 70, 90	0.5
AMTEL	40, 70	50, 80	0.21
Daimler Chrysler	156	80	
Hitachi	76	180	0.25
IBM	47	50	0.35
IBM	48, 90	72, 105	0.18
Infineon	75	80	0.25
Lucent	72	116	0.25
Motorola	48, 75	100, 65	0.25
National Semiconductor	30		0.35
NEC	73	61	0.18
Philips	45	43	
ST Micro	52	71	0.35
Texas Instrument	50		0.35

tions) determined for heterosystems with a steplike transition from the substrate to the film and conducive to a high resulting density of threading dislocations (10^7–10^{10} cm^{-2}) is impaired. As a result, an opportunity arises to control each of these parameters separately, which makes it possible to reduce the threading-dislocation density to a value smaller than 10^5–10^6 cm^{-2}.

4. ELECTRICAL PROPERTIES OF SIGE FILMS ON ARTIFICIAL SUBSTRATES

First of all, we should mention the continuing and growing use of the GeSi solid solution in so-called heterostructure bipolar transistors (HBTs) based on GeSi/Si heterostructures. It is evident that heterostructures without MDs (i.e., with a pseudomorphic base) are necessary for HBTs. It is also noteworthy that the SiGe/Si-based HBTs have been brought into commercial production and more than ten leading companies are already producing (or will be producing in the near future) ultrahigh-frequency integrated circuits based on HBTs. The most important characteristics of Si–Ge HBTs are listed in Table 2 [123]. At present (May 2002), the best characteristics of SiGe/Si HBTs are f_T = 207 GHz and $f_{\max}$ = 285 GHz [124].

The set of electrical parameters for the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ solid solution, which are of interest from the standpoint of device applications (as for any semiconductor), is rather wide. Undoubtedly, the most important of these parameters are the concentration and mobility of free charge carriers. The product of these quantities defines the conductance of the undepleted channel in a metal–oxide–semiconductor (MOS) transistor (or in a field-effect transistor with modulation doping) or the conductance of the base of a HBT; i.e., this product represents one of the most important characteristics of a device. If we consider optoelectronic applications of SiGe/Si heterostructures, we realize that, in this case, the most important parameter (along with the concentration and mobility of the charge carriers) is the concentration of nonradiative-recombination centers related to the point and linear defects in the structure. For example, if the dislocation density in Si and Ge single crystals is lower than 10^6 cm^{-2}, it virtually does not affect the electron and hole mobility; in contrast, the effect of this density on the lifetimes τ_n and τ_p of minority charge carriers is appreciable even if the dislocation density is as low as 10^3 cm^{-2}. Notably, $\tau_n(\tau_p) \sim N_{\mathrm{disl}}^{-1}$ [125], whereas the absolute value of $\tau_n(\tau_p)$ depends heavily on the impurity type and the doping level.

Even more conclusive evidence of the effect of isolated dislocations on the properties of the *n*-Si/*p*-GeSi *p*–*n* heterojunction was obtained in the course of unique *in situ* studies using a transmission electron microscope [126]. Figure 19a shows the dependence of a reverse current on the number of misfit dislocations in the heterojunction plane. Dislocations were introduced into the structure (see the inset in Fig. 19) by heating the sample directly in the column of a transmitting electron microscope; the current–voltage characteristic of the structure (after cooling to 300 K) was also measured *in situ*. Similar correlations were also obtained using traditional methods (Fig. 19b) [127].

4.1. Electrons

A major contribution to the development of the technology for growing Ge_xSi_{1-x} films on an intermediate buffer layer with a varying composition was made by the team of researchers headed by Fitzgerald [30–32, 36, 59]. The fabrication of Ge_xSi_{1-x} solid-solution films with a low dislocation density ($N_{disl} \le 10^6$ cm^{-2}) was originally reported in 1991 [30]. Rapid thermal chemical-vapor deposition was used [30] to grow the films at a substrate temperature of 900°C; the composition gradient in the buffer layers amounted to 10% of the Ge content per micrometer of depth [30]. Unprecedented low densities of threading dislocations were obtained in these structures: $(4 \pm 0.5) \times 10^5$ cm^{-2} for $x = 0.23$ and $(3 \pm 2) \times 10^6$ cm^{-2} for $x = 0.5$. Shortly thereafter, high mobility of electrons in similar layers grown by MBE on a graded buffer layer was reported [128]. A two-dimensional electron gas (2DEG) was formed in a quantum well (QW) fabricated from pure silicon (a 15-nm-thick pseudomorphic Si film) using the method of modulation doping to introduce an Sb donor impurity (~10^{18} cm^{-3}) into the 40-nm-thick $Ge_{0.30}Si_{0.70}$ top layer; a 10-nm-thick spacer made of undoped solid solution with the same composition was used. According to the results of Hall effect measurements in the van der Pauw configuration (assuming that the Hall factor is equal to unity), the 2DEG density was 1.2×10^{12} cm^{-2} at 300 K and 7.8×10^{11} cm^{-2} at $T < 77$ K. The electron mobility in this gas was equal to 9600 cm^2 V^{-1} s^{-1} at 77 K and 96000 cm^2 V^{-1} s^{-1} at 4.2 K.

Over the last ten years, the number of publications concerned with the electrical properties of 2DEG and two-dimensional hole gas (2DHG) in modulation-doped SiGe/Si heterostructures has exceeded several hundred; therefore, we refer the reader to the comprehensive reviews [1, 2, 129–131] which illuminated the current state in this field up to 2000, we will mention only the most important and recent relevant publications.

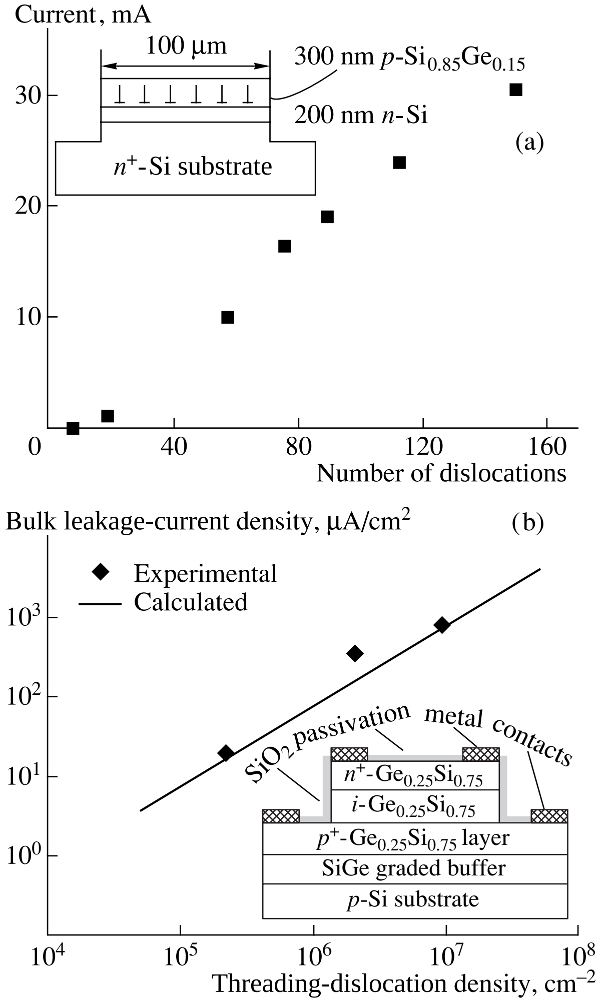


Fig. 19. (a) Dependence of reverse current through the n-Si/p-SiGe heterojunction on the number of misfit dislocations which intersect a 1-cm-long segment of the heteroboundary; the measurements were performed using an electron microscope; the heterojunction was biased by 0.5 V [123]. (b) Dependence of the leakage current in the bulk of the $Si_{0.25}Ge_{0.75}$ p–i–n diode (see the inset) on the density of dislocations threading from the graded-gap buffer layer [124].

The advent of artificial GeSi substrates with a low density of threading dislocations and the use of these substrates to form 2DEG and 2DHG with high mobilities of charge carriers (μ_n = 180000–200000 cm^2 V^{-1} s^{-1} at $T = 4.2$ K and $\mu_p \ge 17000$ cm^2 V^{-1} s^{-1} at $T = 40$ K [132]) necessitated a comprehensive theoretical analysis of scattering mechanisms in the SiGe heterostructure. Monroe *et al.* [133] analyzed the following mechanisms that can limit the low-temperature mobility in a 2DEG: (i) scattering by "remote" donors, which are separated from 2DEG by a spacer made of undoped solid solution; (ii) scattering by background impurities; (iii) scattering at roughness of the heterointerface; (iv) scattering at the fluctuations of the solid-solution composition; and (v) scattering by dislocations penetrating into the channel from a completely relaxed graded-gap buffer layer. Comparison with experimental data made it possible to state [133] that threading dislocations (if their density was lower than 10^6 cm^{-2}) did not limit the mobility in 2DEG (and 2DHG) and that the first four mechanisms were the most important. It was shown [134] that, if the mean amplitude of the heterointerface roughness (to be more specific, the amplitude of the corresponding Fourier component of the roughness spectrum) exceeded 1.2 nm, the electron mobility was no higher than 10^5 cm^2 V^{-1} s^{-1} at $T = 0.4$ K in a 30-nm-thick SI QW with a 2DEG density of 5×10^{11} cm^{-2} (Fig. 20). A similar problem was considered in more detail by Yutani and Shiraki [135]; the dependence of electron mobility on the channel thickness was studied.

Ismail *et al.* [136] noted that the role of misfit dislocations was underestimated by Monroe *et al.* [133].

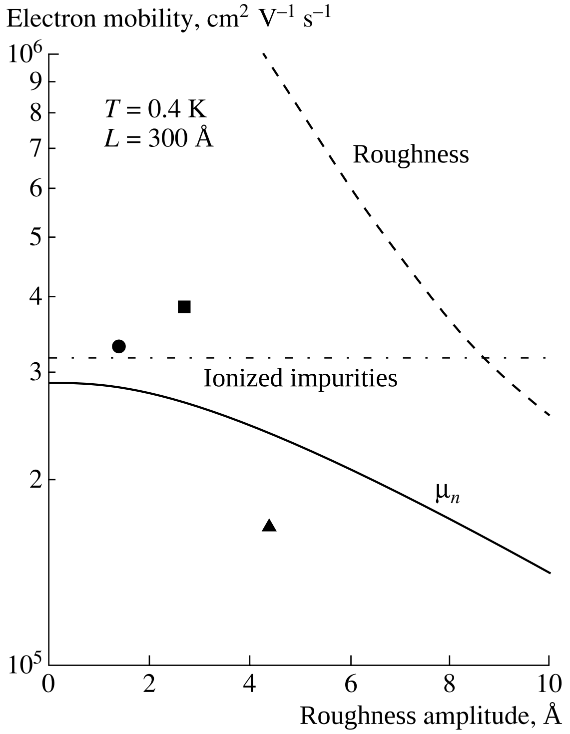


Fig. 20. The electron mobility in pseudomorphic Si films (d = 7–8 nm, n_s = 5–6 × 10^{11} cm^{-3}, T = 0.4 K) grown on thick relaxed buffer layers with the final composition of $Si_{0.7}Ge_{0.3}$ as a function of the roughness amplitude for a heteroboundary with a lateral correlation length of 30 nm. The circle, square, and triangle correspond to experimental data. Theoretical results: dashed line represents the contribution of roughness; the dash-and-dot line, the contribution of scattering by ionized impurities; and the solid line was calculated taking into account both mechanisms.

Ismail *et al.* [136] drew attention to the fact that misfit dislocations (in addition to threading dislocations) could be found at the interface between the SiGe buffer layer and Si channel if the thickness of the channel layer exceeded the critical thickness. Using Ge_xSi_{1-x} buffer layers with a varying final composition (x = 0.34, 0.3, and 0.25) and growing Si films with subcritical and supercritical thicknesses, Ismail *et al.* [136] used transmission electron microscopy to ascertain that MDs were indeed formed at the SiGe/Si interface in accordance with the Matthews–Blakeslee model [7, 14]. The MD generation was accompanied by a decrease in electron mobility in the channel; this effect can be related to the strain field which is generated by 60° MDs and penetrates into the channel.

Ismail *et al.* [136] managed to obtain mobilities in 2DEG at a level of (300–400) × 10^3 cm^2 V^{-1} s^{-1} in structures with a pseudomorphic channel at T = 0.4–1.4 K; if the substrate was used as a back gate, the mobility was even higher (526000 cm^2 V^{-1} s^{-1} at T = 0.4 K). This result remained unsurpassed for a long time until Sugii *et al.* [137] reported an electron mobility of 800000 cm^2 V^{-1} s^{-1} at T = 15 K. The latter mobility is the highest ever achieved. In Fig. 21, we summarize the data [138, 139] on the temperature dependence of electron mobility in modulation-doped pseudomorphic Si channels on artificial GeSi substrates.

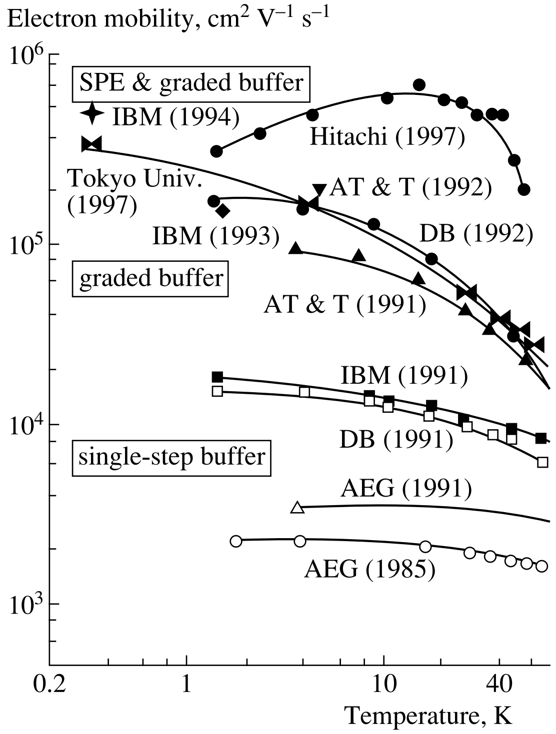


Fig. 21. Chronologically arranged collection of data on the temperature dependence of the Hall mobility for two-dimensional electron gas in pseudomorphic Si films grown on artificial GeSi substrates [135, 136].

The low-temperature mobility of charge carriers is generally of no practical interest but serves as a sensitive indicator of the quality of SiGe/Si heterostructures. The charge-carrier mobility at room temperature or higher (to be more specific, from –60°C to 100°C) is important for practical applications. At these temperatures, the pattern changes significantly and scattering of electrons at the deformation potential of acoustical phonons becomes the main limitation of mobility. Corresponding calculations were carried out by Basu and Paul [140] for a specific structure (a $Si_{0.5}Ge_{0.5}/Si/Si_{0.5}Ge_{0.5}$ QW with an Si layer thickness of 6 and 9 nm on an $Si_{0.75}Ge_{0.25}$ relaxed buffer layer on Si(001) substrate). The calculations showed that the mechanism of intervalley scattering, which is dominant in bulk unstrained silicon, was found to be virtually suppressed in a stretched pseudomorphic Si film; in addition, the conductance of the channel [140] was shown to be governed by electrons with a low longitudinal effective mass (m^* = $0.19m_0$). The combination of these factors in such a film makes it possible to attain an electron mobility which exceeds the mobility in bulk Si by a factor of 1.5–2 (even if the 2DEG density is equal to 1 × 10^{12} cm^{-2}). The predicted effect has been repeatedly substantiated experimentally; an electron mobility exceeding 2000 cm^2 V^{-1} s^{-1} in modulation-doped pseudomorphic Si channels at room temperature is not something extraordinary (keeping in mind that electron mobility in intrinsic Si at 300 K is 1450 cm^2 V^{-1} s^{-1}). The mobility equal to 2830 cm^2 V^{-1} s^{-1} reported in [141] is unprecedentedly high. In one of the recent studies in this field [142], mobility in the channel exceeded that in the bulk material also by a factor of 1.8.

4.2. Holes

The complex anisotropic three-subband structure of the valence-band top in silicon and germanium makes the problem of calculating the kinetic effects in *p*-Si and *p*-Ge extremely difficult even if strains are disregarded [143–145]. Elastic nonuniform strains (at a level of 1%) bring about a radical reconfiguration of constant-energy surfaces of the valence band. By way of example, Fig. 22 shows the constant-energy sections (E = 40 meV) of a heavy-hole band in Si subjected to uniaxial deformation in the [001] direction (panel *a*: 0.7% compressive strain; panel *b*: undeformed state; and *c*: 0.7% tensile strain). Taking into account that there are three types of holes (heavy, light, and those related to spin–orbit coupling), we find that the Hall factor (r_H) in *p*-Si can vary from 3 to 0.1 when the strain along the [001] direction varies from –1 to +1% [146]. Therefore, it is clear that calculation of the hole concentration based on the assumption that $r_H = 1$ may lead to unacceptably large errors. Theoretical approaches to calculating the hole and electron mobilities and the energy-band structure in pseudomorphic [grown on Si(100)] and unstrained $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ solid-solution films are outlined elsewhere (see papers [147–152] and book [153]).

Pseudomorphic SiGe films are used in device structures as materials for modulation-doped QWs with top and bottom layers composed of pure silicon or a solid solution with an increased content of germanium (Fig. 23). In this case, scattering by remote acceptors and at rough heterointerfaces is added to the mechanisms of scattering in bulk SiGe. It has been shown convincingly in a number of publications that scattering at the surface roughness is dominant at low (liquid-helium) temperatures [154]. As of 1995, the highest low-temperature mobility of holes in 2DHG has been 19820 cm^2 V^{-1} s^{-1} at T = 7 K in a modulation-doped “normal” (Fig. 23a) $\mathrm{Si/Si_{0.93}Ge_{0.07}/Si}$ heterostructure (in this case, the sheet concentration of holes is 3.9×10^{10} cm^{-2}) [155].

The charge-carrier mobilities of 1300 cm^2 V^{-1} s^{-1} at 300 K and 14000 cm^2 V^{-1} s^{-1} at 77 K were reported [156] for 12.5-nm-thick Ge channels grown on relaxed buffer layers with a thickness of 3–5 μm and modulation-doped with Ga to a sheet hole concentration of 1×10^{12} cm^{-2}; the structure had a 1.2-μm-long gate and $\mathrm{Si_{0.4}Ge_{0.6}}$ top and bottom layers. This made it possible to fabricate field-effect transistors (FETs) with the slope of the current–voltage characteristic (g_m) equal to 125 and 290 mS/mm at 300 and 77 K, respectively. It is worth noting that FETs with a graded-gap $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ channel (with a thickness of 4.5 nm and with x varying from 0.7 to 0.55) fabricated on artificial $\mathrm{Si_{0.7}Ge_{0.3}}$ substrates by the IBM company [157] are almost as good as the FETs reported in [156] with respect to the slope of the current–voltage characteristic; specifically, the IBM FETs had g_m = 105 and 205 mS/mm at 300 and 77 K, respectively (the channel length was 0.7 μm).

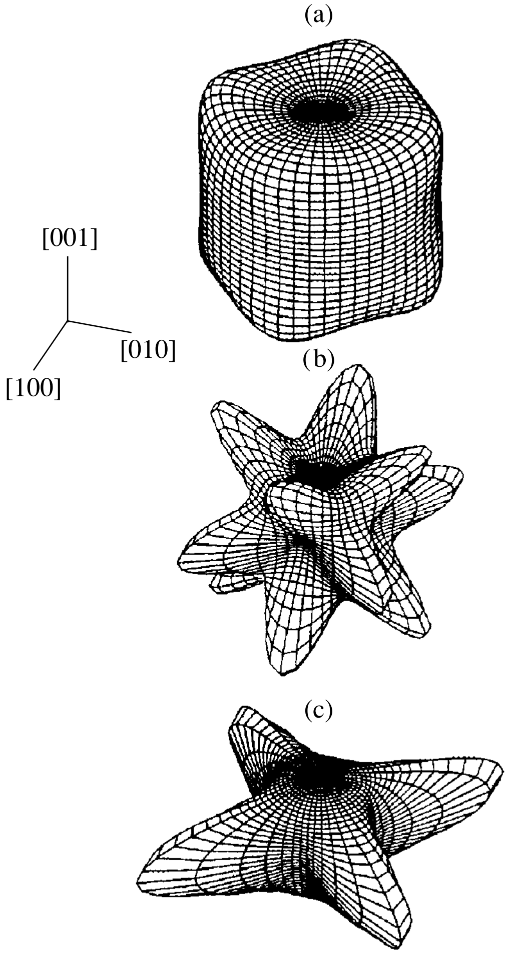


Fig. 22. Constant-energy surfaces (E = 40 meV) for the band of heavy holes in a silicon crystal: (a) a crystal stretched by 0.64% along the [001] direction; (b) an unstrained crystal; and (c) a crystal compressed by 0.64% along the [001] direction (reproduced with permission of the authors [143]).

Structures in which electrical parameters of 2DHG are measured include many layers in addition to the channel with 2DHG (see Fig. 23); these layers may affect the results of measurements. As a result, simple Hall effect measurements are inadequate to correctly determine the charge-carrier mobility. In this situation, the “mobility spectrum” method [158], which accounts for the conductivity of a parallel channel, yields more precise data on the mobility [159]. The Hall mobility

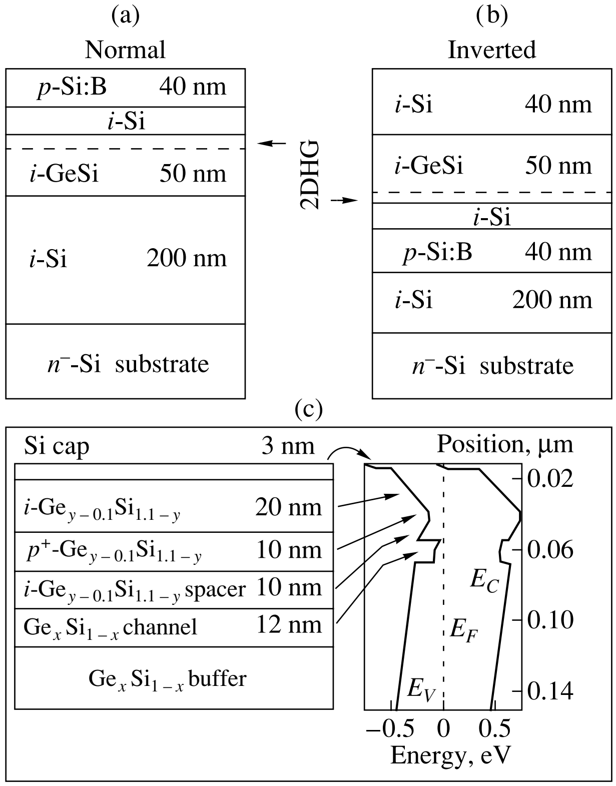


Fig. 23. Cross section of typical heterostructures used in measurements of the charge-carrier mobility in two-dimensional hole gas within pseudomorphic SiGe channels formed on Si substrates [(a) is a normal structure and (b) is an inverted structure)] and also (c) on artificial GeSi substrates [156].

can increase by 50% if parasitic *n*-type conductivities in *i*-type layers are taken into account [159].

As mentioned above, artificial SiGe substrates grown on a buffer layer with a varying composition have a number of serious drawbacks (see Subsection 2.2). One of these drawbacks is related to roughness, which tends to build up as thick (3–10 µm) buffer layers are grown: a typical amplitude of the profile can be as large as 10–15 nm. Over the last decade, numerous efforts have been made to reduce the thickness of the GeSi buffer layer, thus decreasing the roughness of its surface, while retaining an acceptable density of threading dislocations or even reducing it. The method suggested by Chen *et al.* [20] was found to be the most appropriate; this method is based on the use of Si and GeSi buffer layers grown at low temperatures. The electrical parameters of 2DHG in an SiGe/Si heterosystem fabricated using this technology represent the state of the art in this field. In what follows, we consider the relevant results.

Irisawa *et al.* [160] grew $Si_{0.33}Ge_{0.67}$/Ge/$Si_{0.33}Ge_{0.67}$ structures with Ge QWs modulation-doped with B; an $Si_{0.73}Ge_{0.27}$ buffer layer grown at low temperatures was used. The amplitude of the LT-Si surface roughness did not exceed 5 nm. Irisawa *et al.* systematically varied the thickness of the Ge channel (the growth temperature was 350°C) and obtained hole mobilities of 1300 $cm^2 V^{-1} s^{-1}$ (20 K) and 1175 $cm^2 V^{-1} s^{-1}$ (300 K) at a Ge channel thickness of 7.5 nm. A decrease in the growth temperature to 300°C made it possible to obtain a hole mobility of 1320 $cm^2 V^{-1} s^{-1}$ at 300 K. It should be mentioned that the data on hole mobilities of about 1700 $cm^2 V^{-1} s^{-1}$ (300 K) reported previously by Ueno *et al.* [161, 162] were found to be erroneous [160] as a result of incorrect Hall measurements.

Until recently, the highest hole mobility in a pseudomorphic Ge channel (1700 $cm^2 V^{-1} s^{-1}$ at 300 K with $p_s = 7.9 \times 10^{11}$ cm^{-2}) was measured in a $Ge_{0.7}Si_{0.3}$/Ge/$Ge_{0.7}Si_{0.3}$ heterostructure (d_{Ge} = 15 nm) with etched off Si substrate [163]; this mobility is still lower than that in bulk Ge. At the same time, the theory [164] unambiguously predicts a significant increase in the hole mobility in Ge films compressed or stretched along the [001] direction; as a result, the mobility exceeds that in unstrained crystal. As recently as 2002, the mobility-spectrum method was used to ascertain that the hole mobility in elastically strained Ge films is indeed higher than the mobility in an unstressed bulk crystal [165]. Relaxed $Si_{0.33}Ge_{0.67}$ buffer layers were grown in two stages [165]. First, a 50-nm-thick Si layer was formed at 400°C on *n*-Si substrate with a resistivity of 5–10 Ω cm; a 500-nm-thick $Si_{0.73}Ge_{0.27}$ film was then grown on this layer at 600°C. Next, a 50-nm-thick layer with the same composition was grown at 300°C and overgrown at 500°C with a 500-nm-thick $Si_{0.33}Ge_{0.67}$ layer. Finally, a SiGe film doped with B to a concentration of $\sim 2 \times 10^{18}$ cm^{-3} was grown epitaxially on top of the above complex system of buffer layers; a 20-nm-thick Ge active layer was then grown on an undoped 20-nm-thick spacer. The hole mobility in the Ge layer at room temperature was 2940 $cm^2 V^{-1} s^{-1}$, with the sheet concentration of the charge carriers being equal to 5.11×10^{11} cm^{-2}. It is clear that the technology used is quite efficient, so that the correctly measured hole mobility in pseudomorphic Ge film exceeds the mobility in a bulk Ge crystal by 55% (the latter mobility is the highest among all semiconductors). A hole mobility of 2700 $cm^2 V^{-1} s^{-1}$ in a similar structure was also attained owing to doping of $Si_{0.3}Ge_{0.7}$ buffer layers with Sb [166]. Lastly, we note that a high hole mobility in an SiGe/Si heterosystem not only improves the high-frequency characteristics of transistors but also facilitates the solution of the so-called “short channel” problem [167, 168].

4.3. Summary

Thus, it is experimentally ascertained at present that the electrical parameters of 2DEG and 2DHG in pseudomorphic Si, SiGe, and Ge layers grown on artificial SiGe substrates, which are optimized with respect to the structure and surface morphology, excel the kinetic properties of electrons and holes in unstrained crystals. Therefore, we may expect that these structures will be widely used in the near future in the electronics of superlarge-scale integration. At the same time, it is also clear that much effort is still needed in order to develop a commercial technology for the fabrication of complementary MOSs; research in this field is being actively pursued [169–171]. Leading researchers at IBM emphasized at the IEEE International Solid-Circuit Conference [172] that the crucial factor for the commercial success of SiGe/Si-based HBTs is the fact that, in their production, it is possible to use the same equipment and the same technological processes as those used in the production of Si integrated circuits. It is not inconceivable that the use of artificial SiGe substrates will make it possible to attain real success in the development of relevant FETs.

5. CONCLUSION

As a result of more than 20 years of studies of the structural characteristics of plastically relaxing constant-composition GeSi layers grown under conventional conditions, it became clear that the density of threading dislocations in these films is unacceptably high. In our opinion, this is caused by the virtually identical dependences of the density of generated misfit dislocations (MDs) and the velocities of propagation of their threading segments in GeSi heterostructures grown under conventional growth conditions on mismatch stresses. In order to reduce the MD generation rate and, at the same time, preserve an acceptable propagation velocity of the already existing threading dislocation segments, a method for growing graded buffer layers has been suggested; the first encouraging results have been obtained using this method. New methods for film growth, which were developed recently, made it possible to extend the separate effect on the generation and propagation (including annihilation) of MDs; as a result, the crystalline quality of the grown GeSi films improved.

Over the last decade, intensive studies of the growth processes of heterostructures were replaced by practical applications of these structures. As a result of this development, we have observed both unprecedentedly high room-temperature mobilities (exceeding those in bulk crystals) of electrons and holes in 2DEG and 2DHG in Si/GeSi heterojunctions and large-scale applications of these structures in the development of FET metal–insulator–semiconductor transistors.

With respect to the so-called “compliant” substrates, it can be considered proven that the mechanism of elastic relaxation in a stressed film due to the sliding of the film over a viscous substrate is effective only at small distances in the mesoscopic range when the film is of the island type. Relaxation of stresses in extended films occurs via the introduction of misfit dislocations and glide of their threading segments.

We still have some unresolved problems. These include

(i) the remaining ambiguity in choosing a specific method for growing the heterostructures with artificial substrates (some of these methods have still not been adequately tested);

(ii) a deficit in experimental data on the determination of specific mechanisms responsible for a decrease in the density of threading dislocations in such heterostructures; and

(iii) the lack of a widely acceptable technology for forming “compliant” substrate.

ACKNOWLEDGMENTS

This study was supported by the Russian Foundation for Basic Research (project nos. 00-02-17461 and 00-02-17638); the Program for Support of Leading Scientific Schools in the Russian Federation (grant no. 00-15-96806), the program “Promising Technologies and Devices for Microelectronics and Nanoelectronics”; and state contracts from the Ministry of Industry, Science, and Technologies of the Russian Federation (contract nos. 37.029.1.1.0032 and 37.039.1.1.0041). This study was also supported in part in the framework of the federal special program “Integration of Science and Higher Education in Russia for 2002–2006” through Novosibirsk State University and the Scientific Training Center “Technology and Physics of Semiconductor Nanostructures” (contract no. I0765).

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Translated by A. Spitsyn