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Heterostructures Ge_xSi_{1-x}/Si(0 0 1) grown by low-temperature (300–400 °C) molecular beam epitaxy: Misfit dislocation propagation

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Abstract

In previous publications [Tuppen and Gibbings, J. Appl. Phys. 68 (1990) 1526; Hull et al., J. Appl. Phys. 70 (1991) 2052; Houghton, J. Appl. Phys. 70 (1991) 2136], the glide velocity of dislocations was analyzed and estimated in GeSi/Si (0 0 1) heterostructures grown at a temperature of 550 °C. The method of growing GeSi films with the use of a low-temperature Si buffer has been developed recently and was not involved in these studies. The present work deals with a more detailed analysis of dislocation propagation velocities in GeSi films grown with the use of the low-temperature Si buffer and those grown at low-temperatures.

The dislocation velocity is estimated by the measuring of the length of misfit dislocations observed in annealed films. Additionally a method for estimating the mean threading dislocation glide velocity is used, which involves the measured threading dislocation density in a particular film and degree of its plastic relaxation directly related to the number of threading dislocations and their glide velocity. It is shown that dislocation glide velocities in heterostructures grown with the use of the low-temperature Si buffer and at low-temperatures are higher than the values predicted by the classical calculations by an order of magnitude.

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1. Introduction

One of the promising methods of obtaining relaxed Ge_xSi_{1-x} films with a low density of

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threading dislocations in the surface layer is the use of a low-temperature buffer layer of silicon (LT–Si) grown on a Si substrate directly before the growth of the GeSi solid solution [1–8]. This method allows growing Ge_xSi_{1-x} films with the threading dislocation density of 10^5–$10^6\,cm^{-2}$ if the value of "x" does not exceed 0.3 [8].

It is known that plastic relaxation of mechanical misfit stresses in GeSi/Si films is mainly initiated by introducing 60° dislocations aligned with inclined glide planes $\{111\}$, which leads to formation of a network of misfit dislocations at the interface. Threading dislocations are genetically coupled with misfit dislocations; they are the dislocation segments that come out to the film surface. Owing to their glide, the misfit dislocation length increases (see, e.g., [9]), and the level of elastic strains in the film decreases. The value of the residual elastic strains is determined by the total misfit dislocation length in the heterointerface and is approximately the same in layers with a high density of "short" misfit dislocations and in layers with a low density of extended misfit dislocations. Obviously, the threading dislocation density is lower in the second case. In our previous work [10], based on indirect data, we concluded that a decrease in the threading dislocation density in heterostructures grown with the use of LT–Si and at low-temperatures could be caused by two reasons: a decrease in the initial misfit dislocation density and an increase in the threading dislocation propagation velocity.

In previous publications [11–18], the dislocation glide velocity was considered in GeSi/Si (001) heterostructures grown at a temperature of 550 °C and annealed at higher temperatures. The method of growing GeSi films with the use of LT–Si has been developed recently [1,2] and was not involved in these studies. The present work deals with a more detailed analysis of the threading dislocation glide velocities in GeSi films grown with the use of LT–Si and those grown at low growth temperatures.

2. Estimate of dislocation glide velocities

Dislocation propagation velocities in stressed GeSi films as functions of temperature and difference in lattice parameters of the film and Si substrate were analyzed by several teams of researchers: Houghton [11], Hull et al. [13–17], LeGoues et al. [12], and Tuppen and Gibbings [18]. Methods of experimental determination of velocities can be classified into several techniques: direct measurement of the dislocation velocity in an electron microscope with the use of video recording [14]; measurement of the length of misfit dislocation traces on the film surface by Nomarski phase contrast optical microscopy, the traces being formed because of threading dislocation motion during short-time annealing of the samples [11,18] and estimation of the mean misfit dislocation path during a certain time of sample annealing [12].

According to the classical concepts [19] adapted to dislocation gliding in a stressed film [11,18], the velocity of an individual dislocation can be formally represented as

$$V_d = V_0(\tau_{eff}/\mu)^m \exp(-E_v/kT), \quad (1)$$

where V_0 is a constant; μ is the shear modulus; E_v is the activation energy of dislocation motion in the form of gliding; based on various data, the value of m ranges from 1 to 2 (see, e.g., [20]); τ_{eff} is the driving force of the relaxation process, the so-called effective or excess shear stress, which depends on the difference in lattice parameters of the film and substrate and on the film thickness [11,18]. The parameter that exerts the most substantial influence on the dislocation glide velocity is the activation energy E_v. It seems to be logical to assume that this quantity changes linearly with x in stressed Ge_xSi_{1-x} films (from 2.2 eV for Si to 1.6 eV for Ge [16,18]). The parameters V_0 and m can be determined on the basis of the measured velocities of separate dislocations at different temperatures of annealing of GeSi films.

The degree of plastic relaxation of the film is determined by the overall action of misfit dislocations whose length increases owing to gliding of their inclined branches (threading dislocations). Let us estimate the mean dislocation glide velocity on the basis of the measured values of film plastic relaxation and threading dislocation density. The rate of plastic relaxation of an annealed stressed film can be determined as an increase in the normalized total misfit dislocation length per unit time. The total misfit dislocation length depends on the number of misfit dislocations and on the threading dislocation glide velocity, because of which the misfit dislocation length increases. Let us have a stressed pseudomorphic GeSi film grown at low-temperatures. Plastic relaxation of such a heterostructure as a function of time in the course of annealing can be written as

$$R(t) = 1 - \varepsilon_r(t)/\varepsilon_0 = \frac{1}{L_0}\int_0^t L(t)\,\mathrm{d}t = \frac{1}{L_0}\int_0^t \rho(t)\bar{V}_{\mathrm{TD}}(t)\,\mathrm{d}t, \qquad (2)$$

where $\varepsilon_r(t)$ and ε_0 are the residual and initial elastic strains of the film, respectively; $\rho(t)$ and $\bar{V}_{\mathrm{TD}}(t)$ are the threading dislocation density and mean dislocation glide velocity, respectively, L is the total current length of misfit dislocations per unit area; L_0 is the misfit dislocation length per unit area in the case of 100% plastic relaxation, i.e., for $R(t) = 1$. Note that the number of threading dislocations is approximately two times higher than the number of misfit dislocations. Expression (2) yields the mean threading dislocation glide velocity

$$\bar{V}(t) = \frac{\mathrm{d}R}{\mathrm{d}t}\frac{L_0}{\rho(t)}, \qquad (3)$$

or, for our case of discrete measurements,

$$\bar{V} \approx \frac{\Delta R}{\Delta t}\frac{L_0}{\rho}. \qquad (4)$$

The total length of misfit dislocations in two orthogonal grids (L_0) can be calculated for the corresponding difference in lattice parameters of the film and substrate (f) as $L_0 = 2f/\boldsymbol{b}_e$, where $\boldsymbol{b}_e$ is the edge component of the Burgers vector of misfit dislocations in the heteroboundary. The measured quantities are the degree of plastic relaxation of the film and the threading dislocation density in the film after each period of annealing.

Expression (1) describes the glide velocity of an individual dislocation in the absence of decelerating factors, which is normally observed at the initial stage of relaxation, when the interaction of dislocations with each other can be ignored [21]. As the fraction of plastic relaxation increases, both velocities (the glide velocity of an individual threading dislocation and the mean velocity of all threading dislocations participating in the relaxation process) become lower because the driving force τ_{eff} determined by residual elastic strains decreases. Moreover, the mean threading dislocation glide velocity decreases to a greater extent because the increasing number of misfit dislocations exerts a blocking action on the motion of individual threading dislocations, in accordance with the model proposed by Gillard et al. [22]. Hence, it would be more reasonable to estimate the dislocation glide velocity at the initial stages of plastic relaxation of GeSi films.

As it follows from the reasoning described above, to estimate the mean threading dislocation glide velocity in a relaxing sample, one should know the changes in the degree of plastic relaxation of the stressed film per unit time and the threading dislocation density in the film in this period. Some results published by Li et al. [3,5], Hull et al. [14,15] on the degree of plastic relaxation (ΔR) and the threading dislocation density (ρ) in GeSi films at the initial stages of relaxation of mechanical stresses and the mean velocities $\bar{V}_{\mathrm{TD}}$ calculated on the basis of these results by Eq. (4) are listed in Table 1. For comparison, the dislocation glide velocities (V_{d}) calculated by Eq. (1) are also given. The calculations by Eq. (1) were performed for $m = 1$ and under the assumption that the activation energy E_{v} depends linearly on x. The prefactor $V_0 = 1.68 \times 10^{10}$ cm/s was calculated on the basis of the experimental data of Tuppen and Gibbings [18].

In the case of a low threading dislocation density typical of GeSi films with $x \leqslant 0.15$, the mean threading dislocation glide velocity calculated by Eq. (4) is approximately equal to the value obtained by Eq. (1) for these conditions. The observed difference is apparently caused by inexact knowledge of the threading dislocation density, which can vary within an order of magnitude (10^4–10^5 cm^{-2}).

For $x > 0.2$, films grown at a standard temperature of 550 °C, normally have a high threading dislocation density [9]. Thus, for instance, sample No. 2 had a threading dislocation density higher than 10^7 cm^{-2} at the initial stage of plastic

Table 1
Parameters of GeSi films borrowed from the literature and the corresponding dislocation glide velocities calculated by Eqs. (1) and (4)

Authors	No	x (%)	h (nm)	T (°C)	ΔR (%)	Δt (s)	τ_{eff} (GPa)	ρ (cm^{-2})	V_{d} (cm/s) by Eq. (1)	$\bar{V}_{\mathrm{TD}}$ (cm/s). by Eq. (4)
Hull et al.	1	15	300	600[a]	0.32	300	0.52	$\sim 10^4$	1.9×10^{-4}	$\sim 6\times10^{4}$
[14,15]	2	25	35	600[a]	0.34	240	0.62	$\sim 10^7$	5.6×10^{-4}	$\sim 1\times10^{-7}$
Li et al.	3	30	100	550[b]	3	200	1	$\sim 10^5$	3×10^{-4}	$\sim 2\times10^{-3}$
[3,5]	4	30	150	550[b]	10	500	0.89	$\sim 10^5$	2.7×10^{-4}	$\sim 6\times10^{-3}$

[a] Annealing temperature.
[b] Growth temperature.

relaxation, and the degree of its plastic relaxation changed little during annealing. The mean threading dislocation glide velocity calculated for this sample by Eq. (4) is more than three orders of magnitude lower than the velocity calculated by Eq. (1). Such a difference can be attributed to interaction between dislocations [22], which is the reason for many threading dislocations to interrupt their motion or to become completely motionless.

For $x > 0.2$, films grown with the use of LT–Si have a threading dislocation density at a level of $10^5\,\mathrm{cm}^{-2}$ [5]. For these films (sample Nos. 3 and 4), the relation of velocities calculated by Eqs. (1) and (4) has the opposite trend: $\bar{V}_{\mathrm{TD}}$ is greater than V_{d} by an order of magnitude (cf. column Nos. 10 and 11 in Table 1). This difference does not seem to be accidental, and an increase in the threading dislocation glide velocity in GeSi films grown with the use of LT–Si can be one of the factors responsible for the low threading dislocation density. In the next paragraphs, we analyze the threading dislocation glide velocities in GeSi films grown at temperatures of 300–350 °C and with the use of LT–Si.

3. Experimental procedure

Epilayers of solid solutions of $\mathrm{Ge}_x\mathrm{Si}_{1-x}$/Si(0 0 1) with $x = 0.28$ and 0.32 were grown using a "Katun" molecular-beam epitaxy machine equipped with a reflected high-energy electron diffractometer. The molecular silicon flux was generated by an electron-beam evaporator, and a crucible source was used for generation of the molecular germanium flux. The high-temperature 50 nm Si (700 °C) and the low-temperature Si (350 °C) buffers were grown on each substrate. The GeSi films were grown at the rate of 0.09 nm/s and were covered by a 5 nm Si cap layer for the surface stabilization during postgrowth annealing. Samples for annealing were prepared by scribing and cleaving along $\langle 1\,1\,0\rangle$ directions. The samples were annealed at temperatures in the range 350–700 °C in a furnace under an Ar or H_2 ambient. For the fast heating or cooling the quartz pedestal with the sample was pulled in or out of the hot zone of the furnace during 1–2 s.

The structural defects and their spatial distribution were studied using transmission electron microscopy (TEM) with a JEM-4000EX (JEOL) electron microscope. TEM objects were prepared as thin foils oriented in parallel to the growth surface (0 0 1) and as cross sections along the plane (1 1 0). The layer compositions and elastic deformations were determined using a three-crystal X-ray diffractometer with a Si (0 0 4) monochromator in the two-crystal record mode. $\mathrm{CoK}_{\alpha1}$ radiation was used to record diffraction reflection curves. Rocking curves were recorded for symmetrical (0 0 4) and asymmetrical (1 1 5), (2 2 4) and (1 1 3) reflections. In case that the initial degree of plastic relaxation was low (~1%), its value was evaluated on the basis of average misfit–dislocation separation on TEM plan-view images. The density of threading dislocations was measured on TEM images and after the selective etching of heterostructures with an optical microscope equipped with a Nomarski device. A dilute

Schimmel's etchant was applied for selective etching [23]. Practically dislocation-free Si wafers were used, which made it possible to consider all etching pits corresponding to the threading dislocations generated during plastic relaxation of heterostructures.

4. Experimental results

4.1. $Ge_{0.32}Si_{0.68}/Si(001)$ (heterostructure A)

The equilibrium critical thickness of introducing misfit dislocations by Matthews for this system is approximately 8 nm [11,24]. Nevertheless, the heterostructure grown at a temperature of 300 °C to a thickness of 200 nm remained pseudomorphic. The heterostructure was cut into individual samples, which were further annealed. To register the initial stages of plastic relaxation of the stressed heterostructure, annealing with different periods was performed in an argon or hydrogen ambient gas at a temperature of 350 °C, which was only 50 °C higher than the growth temperature. The basic conditions of annealing, the measured threading dislocation density and the degree of plastic relaxation of this heterostructure, and the mean threading dislocation glide velocity calculated on the basis of these data are summarized in Table 2.

Fig. 1 shows the X-ray rocking curves of the as-grown and annealed samples of $Ge_{0.32}Si_{0.68}$ heterostructure. The peak of the as-grown sample displays periodic oscillations, the so-called "thickness fringes", which indicate that the stressed film is fairly perfect. After 10 min of annealing, the oscillations disappeared, and the peak itself became wider, which indicated the beginning of plastic relaxation.

Investigations with transmission electron microscopy (TEM) showed that the threading dislocation glide velocities were rather high, despite the low-temperature of annealing equal to 350 °C, and the length of individual misfit dislocations could be measured only in the sample with the minimum annealing time. Fig. 2 shows a typical TEM image of the misfit dislocations ending with threading dislocation branches. An analysis of the cross-sectional micrographs (1 1 0) and planar foils (0 0 1) showed that the misfit dislocations originated on surface inhomogeneities of the relief. More detailed information on the mechanisms of misfit dislocation generation in this system will be given in [25]. The bar chart of the lengths of the misfit dislocations visualized in Fig. 2 is shown in the inset to this figure. It is seen that the maximum half-length of the misfit dislocations exceeds 2.5 μm. With allowance for the misfit dislocation length and annealing time equal to 10 min, the glide velocity of an individual dislocation can be estimated to be 4×10^{-7} cm/s or higher. The presence of primary misfit dislocations of different length indicates that they do not originate simultaneously; this allows us to assume that there exists some incubation period, namely, a period of time necessary to ensure conditions for the nucleation of the first dislocation loop at a new place.

The threading dislocation glide velocity in annealed samples with longer annealing times

Table 2
The density of the threading dislocations, degree of plastic relaxation of the samples of $Ge_{0.32}Si_{0.68}$ heterostructure annealed at 350 °C in argon or hydrogen, and the mean threading dislocation glide velocity calculated by Eq. (4)

Time of annealing (min)	0	10(Ar)	20(Ar)	30(Ar)	30(H_2)	90(Ar)
Threading dislocation density (cm^{-2})	—	$(1.1\times10^8)^a$	—	$(4–8\times10^8)^a$	$(1.0\times10^8)^a$	$(2\times10^9)^b$
Degree of relaxation (%)	0^c	1^d	3^c	9^c	2^d	12^c
$\bar{V}_{TD}$ (cm/s) By Eq. (4)		2×10^{-7}	—	$(1–2)\times10^{-7}$	1.4×10^{-7}	1.4×10^{-8}

[a] Determined from the measurements of the number of threading dislocations per unit area on plan-view TEM images.
[b] Determined from the measurements of the number of threading dislocations on cross-sectional TEM images.
[c] Determined from X-ray rocking curves for reflection ⟨2 2 4⟩.
[d] Determined from the measurements of the total length of misfit dislocations per unit area on plan-view TEM images.

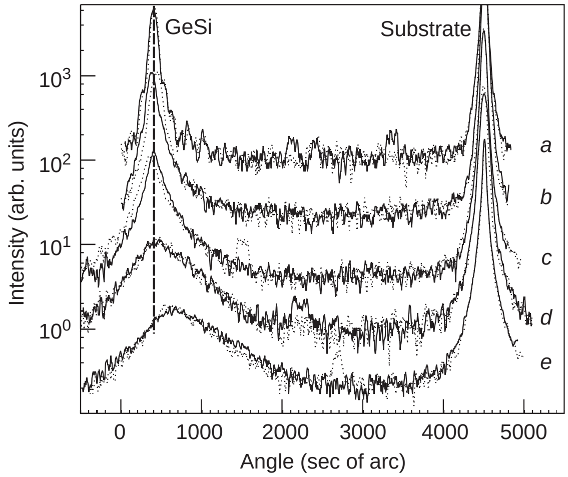

Fig. 1. (0 0 4) X-ray rocking curves for $Ge_{0.32}Si_{0.68}$ heterostructure. The dashed and solid curves in each scan show the two records made with an azimuthal rotation by 180°: (a) as-grown sample, (b–e) after annealing at 350 °C for 10, 20, 30, and 90 min, respectively.

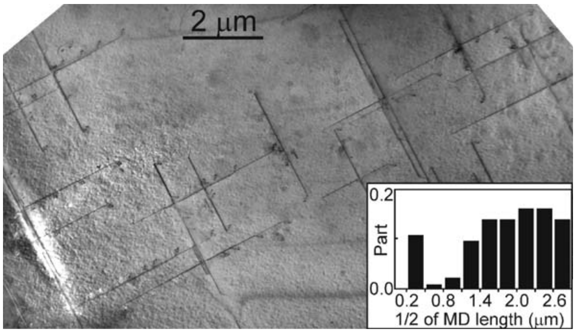

Fig. 2. TEM image of foil of the E9 sample annealed at 350 °C for 10 min. The inset shows the bar chart of the lengths of primary misfit dislocations propagating from the nucleation centers.

(20 and 30 min) was estimated by the maximum length of continuous traces of misfit dislocations observed on the surface near the edge of the film treated in Schimmel's etchant [23]. The edge of the sample is known to be one of the effective sources of dislocations [18] (if the cut is made before heterostructure annealing). In this case, originating at the edge simultaneously with the beginning of annealing, misfit dislocations propagate along the direction ⟨1 1 0⟩ and stop at an identical distance from the edge. Calculating the threading dislocation glide velocity during the time of film annealing, we obtained $V = 9 \times 10^{-7}\,\mathrm{cm/s}$. This value is approximately twice as high as the velocity calculated from the maximum misfit dislocation lengths visible in the electron microscope (Fig. 2). This supports the assumption that there exists an incubation period for generation of misfit dislocations on surface inhomogeneities.

Quantitative processing of images similar to that in Fig. 2 allowed rather accurate measurements of the number of threading dislocations and the total length of misfit dislocations per unit area. Based on these data, we determined the threading dislocation density—$(1.1 \pm 0.2) \times 10^{8}\,\mathrm{cm}^{-2}$ —and the degree of plastic relaxation of this sample after 10 min of annealing—$(R = 1.0 \pm 0.1)\%$. An analysis of plan-view and cross-sectional TEM images allowed us to estimate the relaxation parameters of $Ge_{0.32}Si_{0.68}$ heterostructure annealed for longer times. All results are summarized in Table 2. Based on these data, we calculated the mean threading dislocation glide velocities, which are also listed in Table 2. It is seen that the threading dislocation density increases approximately linearly with increasing time of annealing in argon, which indicates that the rate of misfit dislocation generation is approximately constant. The mean threading dislocation glide velocity remains at a level of $(1\text{–}2) \times 10^{-7}\,\mathrm{cm/s}$ up to $R = 0.09$ and decreases by an order of magnitude in the case of longer annealing and greater degree of plastic relaxation.

It is worth noting that the degree of plastic relaxation and the threading dislocation density in the sample annealed in hydrogen are lower than in samples annealed in argon, other conditions being identical (cf. column Nos. 5 and 6 of Table 2). It is known that hydrogen stabilizes the surface and passivates the surface migration of adsorbed atoms, which, under certain annealing conditions, can lead to surface roughening (well known as two-dimension (2D)—three-dimension (3D) transition) and formation of a microrelief [26]. 3D formation, in turn, favors the origination of heterogeneous surface centers for nucleation of dislocations. Therefore, it can be assumed that the rate of dislocation generation in a stressed structure is lower on a smoother surface. It was this effect that was observed in our case. Annealing in hydrogen similar to annealing in argon in terms of duration and temperature yields a lower degree of plastic relaxation of the film and lower threading dislocation density. At the same time, as is seen from Table 2, the mean threading dislocation glide velocity remains at a level of velocities in samples annealed in argon. This is not a surprise because threading dislocation glide is determined in the first approximation by volume properties of the film, temperature, and values of the acting driving forces.

To analyze the mean threading dislocation glide velocities with deeper plastic relaxation of GeSi films, we annealed the samples of the E9 heterostructure at higher temperatures. To reduce the influence of 2D–3D transformation of the heterostructure surface on formation of new sources of dislocations, annealing was performed in the hydrogen environment. The values of threading dislocation density and degree of plastic relaxation in heterostructure A annealed at temperatures up to 600 °C are given in Table 3. Already after 10 min annealing at 500 °C, the degree of plastic relaxation approaches 80%, and the threading dislocation density determined by analyzing cross-sectional TEM images is close to $10^9\,\mathrm{cm}^{-2}$.

4.2. $Ge_{0.28}Si_{0.72}$/Si(0 0 1) (heterostructure B)

Table 4 contains the basic parameters of $\mathrm{Ge_{0.28}Si_{0.72}}$ heterostructure grown at a temperature of 350 °C with the use of LT–Si and also the calculated mean threading dislocation glide velocity for each annealing temperature. According to X-ray diffractometry, the heterostructure $\mathrm{Ge_{0.28}Si_{0.72}}$ 200 nm thick was pseudomorphic after its growth. The kinetics of plastic relaxation of this heterostructure was examined in the course of isochronous annealing. Based on the TEM data, annealing at 400 °C leads to formation of a regular array of misfit dislocations, formed by sparse bands of the densely packed 60° dislocations. The distance between the bands is more than 1 μm. The

Table 3
The density of the threading dislocations, degree of plastic relaxation of the samples of $\mathrm{Ge_{0.32}Si_{0.68}}$ heterostructure annealed in hydrogen at different temperatures, and the mean threading dislocation glide velocity calculated by Eq. (4)

Temperature of growth or annealing (°C)	300 (growth)	350 (30 min)	400 (10 min)	500 (10 min)	600 (10 min)
Threading dislocation density (cm^{-2})	—	$(1.0\times10^8)^a$	$(1\text{–}2\times10^9)^b$	$(1\text{–}2\times10^9)^b$	$(1\text{–}2\times10^9)^b$
Degree of relaxation (%)	0^c	2^d	40^c	81^c	78^c
$\bar{V}_{\mathrm{TD}}$ (cm/s) By Eq. (4)		1.4×10^{-7}	$4\text{–}8\times10^{-7}$	$1\text{–}2\times10^{-6}$	$8\text{–}16\times10^{-7}$

[a] Determined from the measurements of the number of threading dislocations per unit area on plan-view TEM images.

[b] Determined from the measurements of the number of threading dislocations on cross-sectional TEM images.

[c] Determined from X-ray rocking curves for reflection ⟨2 2 4⟩.

[d] Determined from the measurements of the total length of misfit dislocations per unit area on plan-view TEM images.

Table 4
The density of the threading dislocations, degree of plastic relaxation of the samples of $\mathrm{Ge_{0.28}Si_{0.72}}$ heterostructure annealed in hydrogen during one hour at different temperatures, and the mean threading dislocation glide velocity calculated by Eq. (4)

Temperature of growth or annealing (°C)	350 (growth)	400	500
Threading dislocation density (cm^{-2})	—	$(4\text{–}4.7\times10^6)^a$	$(1\text{–}1.5\times10^6)^a$
Degree of relaxation (%)	0^b	$(2.1)^c$	43^b
$\bar{V}_{\mathrm{TD}}$ (cm/s) Calculation by Eq. (4)		$(1.5\text{–}1.8)\times10^{-6}$	$(1\text{–}1.5)\times10^{-4}$

The threading dislocation density was measured by an optical microscope with the Nomarskii adapter on the surface treated by Schlimmel's etchant.

[a] Determined from etching pits.

[b] Determined from X-ray rocking curves for reflection ⟨2 2 4⟩.

fact that dislocations are grouped into glide bands indicates that, as in the previous case, misfit dislocations were generated by nonexpendable sources associated with the relief of the film surface. The density of these sources, however, was significantly lower because the misfit dislocation lines were very long, whereas threading dislocations were not observed in the images. It is seen from Table 4 that the threading dislocation density was within $5\times10^{6}\,\mathrm{cm}^{-2}$ as a whole; nevertheless, the heterostructure B relaxed by more than 40% already at 500 °C.

5. Discussion

The threading dislocation glide velocities calculated by Eq. (4) and calculated on the basis of the measured misfit dislocation length are compared in Fig. 3 with available reference data, which we consider as the classical results. The solid curves were constructed on the basis of calculations by Eq. (1) for $x = 0.3$ and stressed film thickness of 50 and 200 nm with an allowance of parameters recommended by Tuppen and Gibbinds [18]. The open points are the experimental data of Houghton [11] and Hull et al. [16] for GeSi films with a fraction of Ge close to 0.3. They are in satisfactory agreement with the theoretical dependence. The filled points are our data obtained as described above. The mean threading dislocation glide velocities calculated by Eq. (4) for $Ge_{0.3}Si_{0.7}$/LT–Si/Si(0 0 1) films investigated by Li et al. [3,5] are also given (Table 1). It is seen that all values of both the mean threading dislocation glide velocities and those calculated by the length of individual misfit dislocations in films with the low-temperature buffer layer of silicon and in films grown at low (300–350 °C) temperatures lie above the classical data.

The threading dislocation glide velocity, calculated by the length of individual misfit dislocations in heterostructure A (indicated by the star in Fig. 3) is higher than the dislocation velocity calculated by Eq. (1) by an order of magnitude. The mean calculated velocity $\bar{V}_{\mathrm{TD}}$ for heterostructure A (calculated for samples annealed during 10 and 30 min) was several times lower (rectangle in Fig. 3), which was expected. Nevertheless, this value also exceeds the predicted dislocation velocity for this particular annealing temperature.

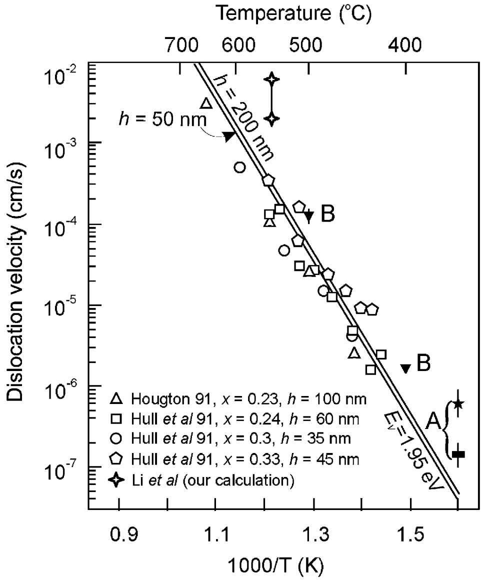

Fig. 3. Threading dislocation glide velocities vs. reciprocal temperature. The solid curves show the calculation by Eq. (1) for $x = 0.3$ and film thickness of 50 and 200 nm. The open points are the experimental data [11,16] for compositions of Ge_xSi_{1-x} films closest to $x = 0.3$. The filled points refer to our data. The mean threading dislocation glide velocities calculated by Eq. (4) for the data of Li et al. [3,5] are also shown.

The mean velocities $\bar{V}_{\mathrm{TD}}$ for heterostructure B annealed at 400 and 500 °C, which were calculated by Eq. (4), were also higher than the predicted dislocation velocity based on classical data. The mean dislocation velocity calculated for sample B annealed at 500 °C should be noted. By the end of annealing, the degree of plastic relaxation of this sample reached 43% (Table 4), which means an almost twofold decrease in excess shear stress τ_{eff} (Eq. (1)). Nevertheless, the mean velocity exceeds the predicted dislocation glide velocity (solid line in Fig. 3) for this temperature.

In Fig. 4 plotted in the same coordinates as Fig. 3, the mean calculated threading dislocation glide velocities for heterostructure A are presented for all annealing temperatures and are connected by lines for convenience. In the case of long-time annealing of the sample (90 min) at a temperature of 350 °C, the mean threading dislocation glide velocity decreases by an order of magnitude (dashed curve in Fig. 4) because, despite a significantly higher threading dislocation density, the degree of plastic relaxation increases only by 3% (last column in Table 2) as compared to that after 30 min annealing. At the same time, with increasing annealing temperature, the mean threading dislocation glide velocity in heterostructure A increases (the corresponding points are connected by the dash and dotted curve), staying above the theoretical dependence approximately up to the 40% degree of plastic relaxation. After that, as the annealing temperature and degree of plastic relaxation increase, the mean threading dislocation glide velocity reaches the saturation level and displays a tendency to decrease, staying noticeably behind the values calculated for the glide velocity of an individual dislocation. The reasons are the decrease in residual elastic strains in the relaxed film and more intense blocking of threading dislocation motion because of compression of the misfit dislocation network (Gillard et al. [22]).

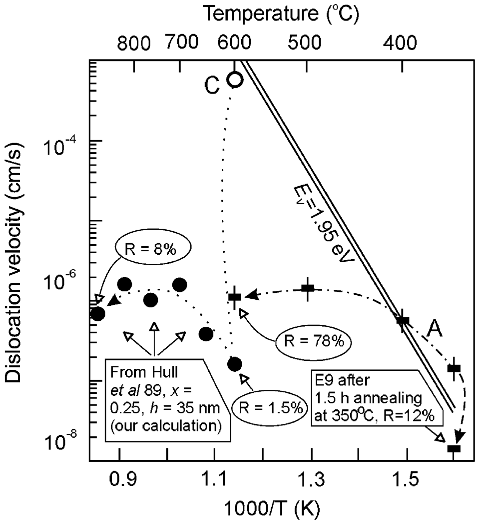

Fig. 4. Mean threading dislocation glide velocities vs. reciprocal temperature, calculated on the basis of data for heterostructure A after annealing at different temperatures (listed in Table 3). The solid curves show the same data as in Fig. 3. The open circle (indicated by C) is the calculated glide velocity of an individual dislocation in the sample from Hull et al. [14]. The hatched circles are the mean threading dislocation glide velocities calculated by Eq. (4) on the basis of parameters of the same sample from Hull et al. [14] after its annealing. The dashed, dotted, and dash and dotted lines are guide to the eye.

The following mechanism leading to an increase in the threading dislocation glide velocity in such films can be assumed. It is known [16] that dislocation gliding occurs due to formation of double kinks on the dislocation line. The double kink dissociates on two single kinks which run along the dislocation line in the opposite directions and the dislocation moves to the neighboring energy valley. Hull et al. [16] showed that only one double kink is formed on the entire dislocation line at each time instant under growth conditions of thin GeSi films with a limited threading dislocation length. If we assume that two or more double kinks are formed simultaneously on the dislocation line, as a result of high density of vacancy clusters [27] in a certain part of the film, this could be the reason for accelerated threading dislocation gliding.

Gillard et al. [22] showed that, in GeSi epilayers with uniform Ge concentration, the strain remaining in the film after relaxation appears to be controlled by the blocking of threading dislocation segments by other misfit dislocations. Relaxation stops when the residual strain is too low to drive threading segments past misfit dislocation. The effect of threading dislocation blocking should be more significant in GeSi films whose thickness is only slightly higher than the equilibrium critical thickness of misfit dislocation introduction. Hull et al. [14] described data on the degree of plastic relaxation and threading dislocation density in a $Ge_{0.25}Si_{0.75}$ film 35 nm thick (the critical thickness is approximately 10 nm [11,24]) for various annealing temperatures up to 950 °C. We used Eq. (4) to treat these data; the mean threading dislocation glide velocity in this film as a function of annealing temperature is shown in Fig. 4 (circles connected by the dotted curve). The calculated glide velocity of an individual dislocation at 600 °C is close to 6×10^{-4} cm/s (Table 1 and the point indicated by C in the beginning of the dashed curve in Fig. 4). The mean threading dislocation glide velocity calculated by Eq. (4), however, was smaller almost by four orders of magnitude already at the initial stage of plastic relaxation. It is seen from Fig. 4 that the mean threading dislocation glide velocity in this sample increases by an order with increasing annealing temperature but remains significantly lower than the data calculated for the corresponding annealing temperatures. The degree of plastic relaxation is also low (within 8% for annealing temperature of 900 °C). In our opinion, such a small increase in the degree of plastic relaxation of this film even at high annealing temperatures is attributed to a rather high-threading dislocation density ($>10^7\,\mathrm{cm}^{-2}$) even at the early stages of stress relaxation. At this threading dislocation density, the processes of interaction between dislocations [22], which decelerate plastic relaxation, play an important role.

Thus, the blocking effect of the network of orthogonally located misfit dislocations, preventing threading dislocation motion, can be quantitatively estimated, namely, it can be characterized by the decrease in the mean threading dislocation glide velocity, as compared to the calculated glide velocity of an individual dislocation.

6. Conclusions

The detailed analysis of dislocation propagation in GeSi films grown with the use of low-temperature Si buffer and those grown at low-temperatures was fulfilled. The dislocation velocity was estimated by the measuring of the length of misfit dislocations observed in annealed films. Additionally the method for estimating mean threading dislocation glide velocity was used. It takes into account the measured threading dislocation density in a particular film and the degree of its plastic relaxation directly related to the number of threading dislocations and their glide velocity. The results obtained were compared with dislocation glide velocities taken from the literature for the GeSi films grown at 550 °C. It was found that the dislocation glide velocities in heterostructures grown with the use of LT–Si and at low-temperatures were higher by an order of magnitude than the values predicted by the classical calculations for these temperatures.

To grow heteroepitaxial films with a maximum degree of plastic relaxation and a minimum density of threading dislocations, one has to ensure growth conditions with a minimum number of heterogeneous centers of dislocation nucleation and a maximum mobility of gliding dislocations. Taking into account the experimental data described above, it can be argued that such conditions for GeSi films are provided by low-temperature (350–400°) molecular beam epitaxy with the use of LT–Si buffer layers.

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