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Analysis of the Stress Relieving Process in a Semiconductor Heterosystem with a (013) Interface

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Abstract—A theoretical analysis of the process of introducing misfit dislocations into a semiconductor heterostructure with a (013) interface is performed by assuming conditions of quasi-equilibrium process. The mechanism of generation is established for those misfit dislocations, which do not meet the requirement of minimum critical film thickness. The calculations are performed on the basis of the force balance model and allow for the shear stress field in the film and the type of the screw dislocation component.

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INTRODUCTION

According to investigations of misfit dislocations (MDs) in semiconductor heterosystems with small mismatch parameter *f*, these dislocations are normally found in slip systems ⟨110⟩{111}. Relaxation of the misfit stresses is possible in the case of 12 slip systems. All families of dislocations have the same Burgers vector magnitude $\boldsymbol{b}$. At a nonsingular interface, each *i*th system has corresponding critical film thickness h_K^i, above which MDs of a given system become energetically advantageous. In this work, two standard ways of computing h_K^i [1, 2] are used in an unconventional analysis of the relaxation process that considers the effect of the shear stress field produced by the relaxation process. It is known that screw dislocation components can be either right or left. Our analysis allows for the effect of the type of MD screw component on the process.

TWO APPROACHES TO CALCULATING A FILM'S CRITICAL THICKNESS

The first approach to describing MD formation is to determine the τ_b values that represent projections of the shift stresses in the slip plane on dislocation Burgers vector $\boldsymbol{b}$. They determine force F_R acting on the threading dislocation formed during relaxation [1]. Generally, $F_R = (hb\cos\lambda)\tau_b$, where λ is the angle between $\boldsymbol{b}$ and the perpendicular to an MD lying in the heterojunction plane. The maximum value of F_R corresponds to the minimum value of the critical film thickness. With a (001) interface, we can write $\tau_b = \sigma^{(0)}(\sin\lambda\cos\theta)$. Here, $\sigma^{(0)}$ represents stresses in the pseudomorphic film and θ is the angle between the dislocation slip plane and the interface. Product $(\sin\lambda\cos\theta)$ is known in the literature as the Schmid factor.

In the second approach [2], critical film thickness h_K^i of the *i*th family is defined as the minimum thickness at which equality is reached between F_R and the linear MD strain, which is given by $F_L = \mu b^2(1 - \nu\cos^2\alpha)(1 + \ln(h/b))/[4\pi(1 - \nu)]$. Here, μ and ν are respectively the shear modulus and the Poisson coefficient of the film, and α is the angle between $\boldsymbol{b}$ and MD. Values of h_K^i are determined from transcendence equation $h_K^i = b(1 - \nu\cos^2\alpha)(1 + \ln(h_K^i/b))/[8\pi f\cos\lambda(1 + \nu)]$, which contains an unknown quantity in both parts.

Both approaches yield identical sets of solutions for h_K^i. With a (013) interface, each set contains six different values presented for the CdHgTe/CdTe(013) structure in [3]. Heterostructures of this type find application in technology. Let us consider the relaxation process under quasi-equilibrium conditions, as exemplified by a $Cd_{0.22}Hg_{0.78}Te$/CdTe(013) heterostructure with mismatch $f = 0.0024$. To families MD_1 and MD_2 (when $\alpha = 79.11°$, $\lambda = 44.18°$, and $\theta = 43.09°$) correspond two equal minimum values $h_K^{1,2} = 41.8$ nm. At the heterointerface, these dislocations are parallel to directions [2 3 −1] and [2 −3 1], respectively. The angle between these directions is $\omega = 64.62°$. Since $\omega \neq 90°$, it is impossible to completely relieve the misfit stresses within the two families of dislocations [4, 5]. We must therefore call on two more families, MD_3 and MD_4 ($\alpha = 40.89°$, $\lambda = 61.44°$, $\theta = 43.09°$), with two more values of $h_K^{3,4} = 51.9$ nm calculated using the models presented in [1, 2]. It should be

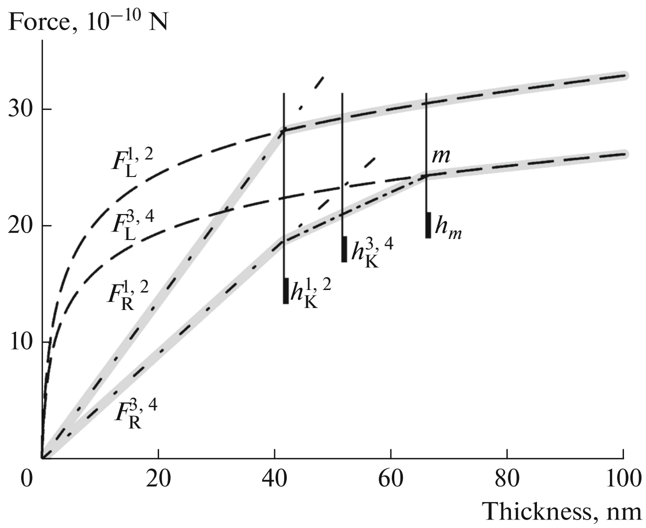

Fig. 1. Dependence of the linear tension forces F_L acting on misfit dislocations and dependence of the forces F_R acting on threading dislocations associated with the MDs on the film thickness h. Heavy lines show the behavior of dependences $F_R^{1,2}(h)$ and $F_R^{3,4}(h)$ throughout the whole process.

noted that both $h_K^{1,2}$ and $h_K^{3,4}$ are determined for a pseudomorphic (i.e., dislocation-free) state of the film.

EFFECT OF THE SHEAR STRESS FIELD AND THE SCREW DISLOCATION COMPONENT ON RELAXATION PROCESS

The analysis performed in this work assumes that the relaxation process involves those MD families in which forces F_L and F_R are equal at a given film thickness. Under quasi-equilibrium conditions, plastic relaxation begins with the introduction of $MD_{1,2}$, since $h_K^{1,2} < h_K^{3,4}$. When an MD is introduced, the stress field in an epitaxial film is described by tensor $\underline{\sigma} = \underline{\sigma}^{(0)} + \underline{\sigma}_\Sigma$, where $\underline{\sigma}_\Sigma = \underline{\sigma}^{(1)} + \underline{\sigma}^{(2)} + ... + \underline{\sigma}^{(n)}$ is the total stress tensor of all MDs that have already formed. Nonzero components of tensor $\underline{\sigma}^{(0)}$ in a pseudomorphic film are equal to $\sigma_{xx}^{(0)} = \sigma_{yy}^{(0)} = \sigma^{(0)} = 2fG(1 + \nu)/(1 - \nu)$. The analytical form of the $\underline{\sigma}$ tensor's components can be written only for long-range stresses caused by the introduction of MD families [4, 5]. The tensor of stresses induced by any family is written in a system of coordinates in which $0x$ is the direction of the MD lines of this family; $0y$ is perpendicular to the MD line lying in the heterointerface plane, and $0z$ is the normal to the interface plane. Taking into account [1, 4–6], for the ith family, the components of long-range stresses of tensor σ_i are equal to $\sigma_{xx}^{(i)} = 2\nu Gb\cos\lambda/(D_i(1 - \nu))$; $\sigma_{yy}^{(i)} = 2Gb\cos\lambda/(D_i(1 - \nu))$ and $\sigma_{xy}^{(i)} = \sigma_{yx}^{(i)} = Gb\cos\alpha/D_i$. Here, D_i denotes the average distance between dislocations for the ith MD family. Tensor $\underline{\sigma}$ is obtained after all tensors $\underline{\sigma}_i$ are reduced to one coordinate system and summed with $\underline{\sigma}_0$. For $\underline{\sigma}$ reduced to the main directions, the half-sum of diagonal components $\sigma_H = (\sigma_{xx} + \sigma_{yy})/2$ describes residual normal stresses in the film, and their half-difference $\sigma_C = (\sigma_{xx} - \sigma_{yy})/2$ describes the value of shear stresses. The degree of plastic relaxation of an epitaxial film can be defined as $\rho = 1 - \sigma_H/\sigma^{(0)}$.

In the classical presentations of MD theory [1, 2], inequality $h_K^{1,2} < h_K^{3,4}$ means that throughout the relaxation process, there are more advantageous conditions for introducing dislocation families MD_1 and MD_2 than for MD_3 and MD_4. This contradicts the results obtained on the basis of our analysis of the quasi-equilibrium relaxation process. In this work, we established there is such a value of h_m that when $h_K^{1,2} < h < h_m$, equality $F_L = F_R$ is fulfilled only for MD_1 and MD_2, When $h > h_m$, it is true for all families MD_1 through MD_4. This means that when $h < h_m$, only the introduction of MD_1 and MD_2 is possible, while when $h > h_m$, the introduction of any of the four dislocations families is possible. Figure 1 shows the results from simulating the process. For $MD_{1,2}$ and $MD_{3,4}$, the logarithmic dependences of linear strain forces on h are denoted as $F_L^{1,2}$ and $F_L^{3,4}$, and the forces acting on the threading dislocations are denoted as $F_R^{1,2}$ and $F_R^{3,4}$. Dependences $F_L^{1,2}$ and $F_R^{1,2}$ intersect at critical film thickness $h_K^{1,2}$. When $h > h_K^{1,2}$, dependence $F_R^{1,2}$ coincides with $F_L^{1,2}$.

The curves of $F_L^{3,4}(h)$ and $F_R^{3,4}(h)$ intersect at $h_K^{3,4}$, the quantity that characterizes the critical thickness of a pseudomorphic film for the introduction of $MD_{3,4}$. Since type $MD_{1,2}$ dislocations are already present in the film starting at a thickness of $h_K^{1,2}$, the film is not pseudomorphic when $h > h_K^{1,2}$. On the threading dislocations of families 3 and 4, an additional force is exerted by the field of stresses produced by MD_1 and MD_2. As a result, the increase in force $F_R^{3,4}(h)$ slows, and the actual critical film thickness for introducing $MD_{3,4}$ becomes h_m, which is the horizontal coordinate of point m. When $h > h_m$, the generation of dislocations MD_3 and MD_4 becomes energetically advantageous in parallel with introduction of MD_1 and MD_2. In the range of thicknesses $h_K^{1,2} < h < h_m$ there is equality only between forces F_L and F_R, determined for MD_1 and MD_2. In the range of thicknesses $h > h_m$, however, the equality between the forces is fulfilled for all four families MD_1–MD_4.

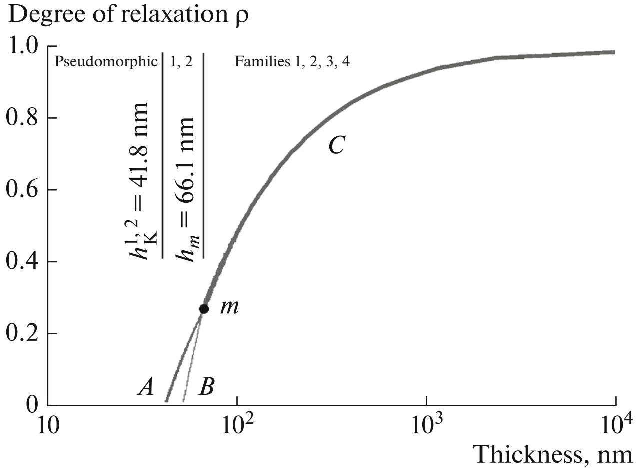

Fig. 2. Dependence of the degree of plastic relaxation $\rho(h)$ at the equilibrium introduction of MD_1, MD_2 (curve *A*) and the introduction of MD_1–MD_4 (curve *C*), along with the dependence on ρ of the critical thickness for introducing MD_3 and MD_4 into an interface containing MD_1 and MD_2 (curve *B*). Epitaxial $Cd_{0.22}Hg_{0.78}Te$ film on a CdTe(013) substrate.

Relationships $\rho(h)$ are shown in Fig. 2 as curves *A*, *B*, and *C*. Curve *A* describes the introduction of $MD_{1,2}$; curve *B*, the change in the critical thickness for the generation of the first dislocation of MD_3 or MD_4 families under conditions of increasing $MD_{1,2}$ density. The lower point of curve *B* coincides with value $h_K^{3,4}$. As the density of families $MD_{1,2}$ grows, the residual normal stresses (denoted earlier as σ_H) are reduced, resulting in monotonic relief of stresses τ_b for all families MD_1–MD_4. However, the shear stresses (denoted above as σ_C) increase. Families MD_1 and MD_3 (as along with MD_2 and MD_4) belong to opposite types of screw components. Because of the effect of shift stresses, force F_R therefore grows faster for $MD_{3,4}$ than for $MD_{1,2}$ as *h* rises. This continues up to the moment when (at point *m*) $F_L^{3,4}$ and $F_R^{3,4}$ become equal. Point *m* in Fig. 2 is the intersection of curves *A* and *B*, and the beginning of curve *C* characterizing the introduction of all four families MD_1–MD_4. Curve *C* was obtained for $D_1 = D_2$ and $D_3 = D_4$ under the condition that in each family there is equality between driving force F_R and force F_L of linear strain. The coordinates of point *m* in Fig. 2 are $h_m = 66.1$ nm and $\rho_m = 0.263$. In Fig. 1, they are $h_m = 66.1$ nm and $F_m = 2.4 \times 10^{-9}$ N.

Calculations show that in a film of the $Cd_{0.22}Hg_{0.78}Te$/CdTe(013) heterosystem average level σ_C of shift stresses builds up to a maximum value of 16 MPa in the region $0 \le \rho \le \rho_m$. In the region $\rho_m \le \rho \le 1$, this level approaches zero.

CONCLUSIONS

Characteristics of the process of introducing MDs into a $Cd_{0.22}Hg_{0.78}Te$ film on a CdTe (013) substrate are generally for an arbitrary semiconductor heterostructure with a (013) interface. The quasi-equilibrium relaxation process is accompanied by the successive introduction of families $MD_{1,2}$ and $MD_{3,4}$ at corresponding critical thicknesses determined by different methods. This results in the accumulation and subsequent removal of shear stresses $\sigma_C = (\sigma_{xx} - \sigma_{yy})/2$ in the epitaxial film. The maximum of this stress is observed at h_m, the critical film thickness for introducing $MD_{3,4}$ into an epitaxial film containing an equilibrium density of $MD_{1,2}$.

As was shown in [4], in the final stage of the relaxation process, the shear stress field is normally $\sigma_C = 0$. It was established in [5] that with singular orientations (001) and (111), condition $\sigma_C = 0$ can be met for all stages of the relaxation process. In this work, it was shown for the first time that nonzero field σ_C inevitably arises when misfit stresses are relieved under quasi-equilibrium conditions at a (013) interface. To what extent this is true for other, nonsingular orientations of the semiconductor crystal lattice will be the subject of further studies.

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