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Reducing the density of threading dislocations in GaAs epitaxial layers. Efficiency assessment of isovalent Bi doping and Pb doping

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Processes of motion of threading dislocations associated with isovalent doping of epitaxial layers were considered. An exact solution was obtained for the gliding distance of dislocations under strains. It was shown that the effectiveness of doping for reducing the density of threading dislocations in an epitaxial layer depends on the product of the surface density of the dislocations in the substrate and the lateral size of the substrate. An analysis of the effectiveness of isovalent Bi doping and standard Pb doping in reducing the density of threading dislocations in GaAs epitaxial layers and the range of applicability has been presented.

Key words: *isovalent doping; dislocations; GaAs; Bi; Pb*

1. Introduction

Dislocations are well known to increase the leakage currents and to degrade the electrophysical parameters of semiconductor devices [1, 2]. The mechanisms of the formation of dislocations in homoepitaxial layers obtained by the liquid phase epitaxy (LPE) are the inheritance of dislocations from the substrate and the difference between the lattice constants of the substrate and the doped epitaxial layer at the growth temperature [3]. Isovalent doping is one of the ways to substantially reduce the dislocation density in GaAs in comparison with the epitaxial layers grown from gallium solution melts [4–8.] The decrease in the dislocation density occurring when Ga based solution melts are replaced by Bi based melts can be explained by an increase of the threshold

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strain associated with the dislocation nucleation [4, 5]. Another explanation for the reduction in the dislocation density in GaAs epitaxial layers doped with indium is a decrease in the supersaturation of vacancies in the elastically strained layer, considerably decreasing the rate of dislocation formation due to vacancy condensation [6].

However, strains in the epitaxial layer enable threading dislocations to glide along the glide planes. The decrease in the density of threading dislocations in the epitaxial layer due to the strains was considered by Matthews, Blakeslee, and Mader [9]. Strains in epitaxial layers result in the appearance of the Peach–Koehler forces (PKF) [10] affecting threading dislocations. Under the PKF, the dislocation can be removed from the epitaxial layer to its edge by gliding resulting in the formation of edge misfit dislocations. The decrease of the number of threading dislocations due to their motion under strain has also been considered by Romanov et al. [11]. The aim of the present paper is a theoretical justification of conditions providing an effective reduction in the density of threading dislocations due to doping GaAs with Bi and Pb.

2. Mathematical model

The model proposed by Martisov [8] was used to analyse the decrease in the dislocation density in the epitaxial layers. The model is based on the balance of the PKF, the force F_1, affecting the inclined part of the threading dislocation in the epitaxial layer, and the force of linear tension of the dislocation, F_2, at the substrate/epitaxial layer interface plane, being the part of the edge misfit dislocation (Fig. 1).

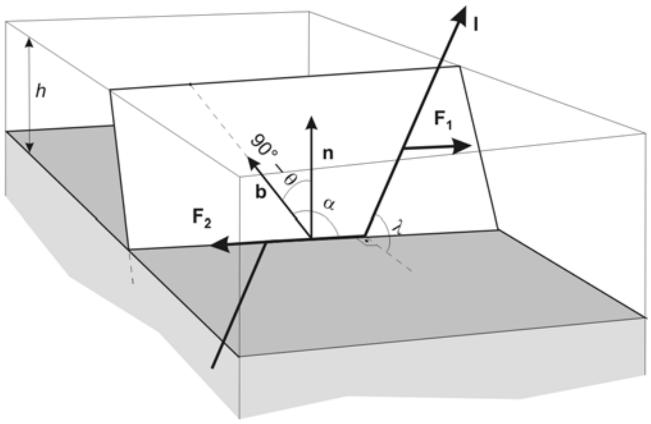

Fig. 1. Schematic diagram of the strained epitaxial layer on the substrate with a threading dislocation moving along its glide plane

The PKF arises in the strained layer and is defined by the following expression [10]:

$$dF_1 = -\mathbf{l} \times (\mathbf{b} \cdot \tau) dl \tag{1}$$

where **l** is the unit vector along the dislocation line, **b** is the Burgers vector, $\boldsymbol{\tau}$ is the tensor of stress field, and *dl* is the increment of the dislocation length, respectively.

For the analysis, it has been assumed that:

- Both the substrate and the epitaxial layer are isotropic media.
- The stresses caused by the misfit *f* of the lattice constants corresponding to the substrate and to the epitaxial layer are distributed uniformly in the substrate/epitaxial layer interface plane.
- There is no interaction between the dislocations.
- Threading dislocations in the epitaxial layer are inherited from the substrate and their density is equal to the surface density of the dislocations in the substrate.

Under these assumptions, the projection of the PKF on the slip plane and the modulus of the force of the linear tension of dislocation are defined by the following expressions [12, 13]:

$$F_1 = \frac{2G\varepsilon bh(1+\nu)}{1-\nu}\cos\lambda \tag{2}$$

$$F_2 = \frac{Gb^2}{4\pi(1-\nu)}\left(1-\nu\cos^2\alpha\right)\left(\ln\frac{h}{b}+1\right) \tag{3}$$

where G is the shear modulus, ε is the elastic stress in the epitaxial layer, b is the magnitude of the Burgers vector, h is the thickness of the epitaxial layer, ν is the Poisson ratio, λ is the angle between the slip direction and the direction in the substrate/epitaxial layer interface plane that is perpendicular to the line of intersection of the slip plane and the interface, and α is the angle between the dislocation line and the Burgers vector, respectively.

The dislocation starts to move in the slip plane when $F_1 > F_2$ and accommodates the misfit δf due to the formation of a part of the purely edge misfit dislocation. The misfit δf can be calculated as follows, assuming that dislocations do not interact [8]:

$$\delta f = qN_d Lb\cos\theta \tag{4}$$

where θ is the angle between the Burgers vector and the interface, the multiplier q takes into account the existence of equivalent slip directions and, hence, reduction of the density of the slipping dislocations along concerned direction, $q \le 1$, N_d is the surface density of the dislocations in the substrate. Vector **n** in Fig. 1 is the normal vector to the substrate/epitaxial layer interface. The strain in the structure is calculated as follows:

$$\varepsilon = f - \delta f = f - qN_d Lb\cos\theta \tag{5}$$

Equating F_1 with F_2 (Eqs. (2) and (3)) and substituting the expression for the strain (5) in (2), the distance passed by the threading dislocation under the driving force can be calculated as follows:

$$L = \frac{1}{qN_d b\cos\theta}\left(f - \frac{b}{8\pi h(1-\nu)\cos\lambda}\left(1-\nu\cos^2\alpha\right)\left(\ln\frac{h}{b}+1\right)\right) \tag{6}$$

As follows from Eq. (6), at a certain thickness h_c of the epitaxial layer, L can be longer than the characteristic lateral size of the substrate D. Under such conditions dislocation is removed from the epitaxial layer to the edge of the structure. Equation (6) can be solved exactly, with respect to the thickness of the epitaxial layer, using the approach proposed by Braun et al. [14].

Rewriting Eq. (6) as

$$\frac{(f - qLN_d b\cos\theta)\times 8\pi(1+\nu)\cos\lambda}{\left(1-\nu\cos^2\alpha\right)}\frac{h}{b} = 1 + \ln\left(\frac{h}{b}\right) \tag{7}$$

and substituting

$$A = -\frac{(f - qLN_d b\cos\theta)\times 8\pi(1+\nu)\cos\lambda}{e\left(1-\nu\cos^2\alpha\right)}, \qquad X = \frac{h}{b}e$$

the following equation is obtained:

$$AX + \ln X = 0 \tag{8}$$

Let

$$X = \frac{1}{A}W(A)$$

with $W(A)$ being a certain function. Then Eq. (8) can be rewritten as follows:

$$\mathrm{W}(A)\mathrm{e}^{W(A)} = A \tag{9}$$

The function $W(A)$, called the Lambert W function [16], is a complex and multi-valued function with an infinite number of branches, only two of them having real values. The real branches of the Lambert W function are shown in Fig. 2. It is necessary to ascertain which of the two branches corresponds to a correct physical solution.

The absolute value of A decreases with the increase of the accommodation of misfit between the lattice constants of the substrate and the epitaxial layer due to the spreading of the dislocations. With the increase of the thickness of epitaxial layer, the projection of the PKF on the slip plane also increases. Hence, the equality of forces F_1 and F_2 is achieved at smaller residual strains in the epitaxial layer. Based on the fact that A is always negative and the value of X decreases as the absolute value of A increases, the physical solution corresponds to the positive value of dX/dA.

Using the expression for the derivative of the Lambert *W* function, which can be easily obtained by differentiation of Eq. (9)

$$\frac{dW(x)}{dx} = \frac{W(x)}{x(1+W(x))}$$

the following expression can be obtained:

$$\frac{dX}{dA} = -\frac{1}{A^2}\frac{W^2(i,A)}{1+W(i,A)}, \qquad i = 0, -1$$

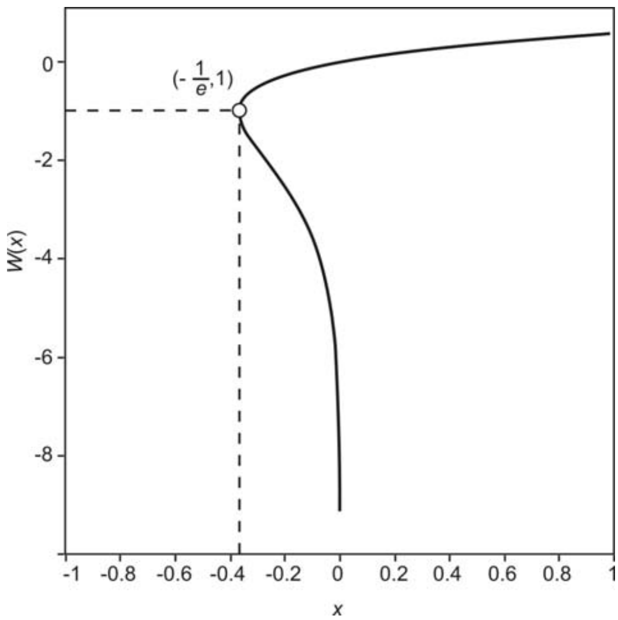

Fig. 2. The real valued Lambert *W* function with two branches, *W*(0, *x*) and *W*(–1, *x*)

As can be seen from Fig. 2, only the derivative of the function *W*(–1, *x*) is positive.

The solution of Eq. (6) with respect to the thickness of the epitaxial layer *h* can be written as follows:

$$h = -b\frac{(1-\nu\cos^2\alpha)}{(f-qLN_d b\cos\theta)\cdot 8\pi(1+\nu)\cos\lambda} \times W\left(-1, -\frac{(f-qLN_d b\cos\theta)\cdot 8\pi(1+\nu)\cos\lambda}{e(1-\nu\cos^2\alpha)}\right) \qquad (10)$$

The value of the critical thickness h_c is calculated as follows:

$$h_c = -b\frac{\left(1-\nu\cos^2\alpha\right)}{\left(f-qDN_d b\cos\theta\right)\times 8\pi\left(1+\nu\right)\cos\lambda} \times \mathrm{W}\left(-1,-\frac{\left(f-qDN_d b\cos\theta\right)\times 8\pi\left(1+\nu\right)\cos\lambda}{e\left(1-\nu\cos^2\alpha\right)}\right) \quad (11)$$

3. Results and discussion

Equation (11) can be applied to estimate the effectiveness of isovalent doping of GaAs by Bi and doping by Pb for the removal of threading dislocations from the inner epitaxial layer to its edge, due to the formation of edge misfit dislocations.

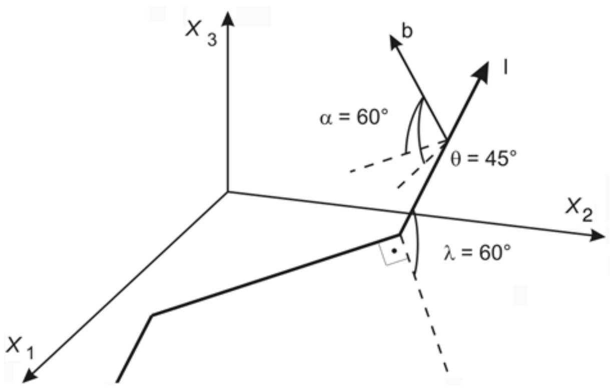

Fig. 3. Motion of the threading 60° dislocation in the strained epitaxial layer with the direction of the inclination of the dislocation line

It is known that {111} planes are the slip planes in GaAs. Consider the dislocation with 60° inclination having the direction $\mathbf{l} = 1/\sqrt{2}\,[011]$ and the Burgers vector $\mathbf{b} = a/2$ [101]. Such dislocations have been reported elsewhere [16, 17]. Then α = 60°, λ = 60°, and θ = 45° (see Fig. 3). Since there are two independent directions of the dislocation spread, namely $\mathbf{l}_1 = 1/\sqrt{2}[011]$ and $\mathbf{l}_2 = 1/\sqrt{2}[0\bar{1}1]$ [8, 9], the value of q is 1/2.

The misfit f can be defined as [8]:

$$f = 1-\left(\frac{1+\left(\frac{M_{\mathrm{dop}}}{M_{\mathrm{sub}}}-1\right)x}{1+\left(\frac{\rho_{\mathrm{dop}}}{\rho_{\mathrm{sub}}}-1\right)x}\right)^{1/3} \quad (12)$$

where M_{sub}, M_{dop}, ρ_{sub}, ρ_{dop} are the molar masses and the densities of materials of the substrate and the dopant, respectively, x is the molar fraction of the dopant in the substrate which can be calculated using the following expression [8]:

$$C_{dop} = \frac{N_A x}{\dfrac{M_{sub}}{\rho_{sub}}(1-x) + \dfrac{M_{dop}}{\rho_{dop}}x} \tag{13}$$

Here, C_{dop} is the concentration of the dopant in the epitaxial layer and N_A is the Avogadro number, respectively.

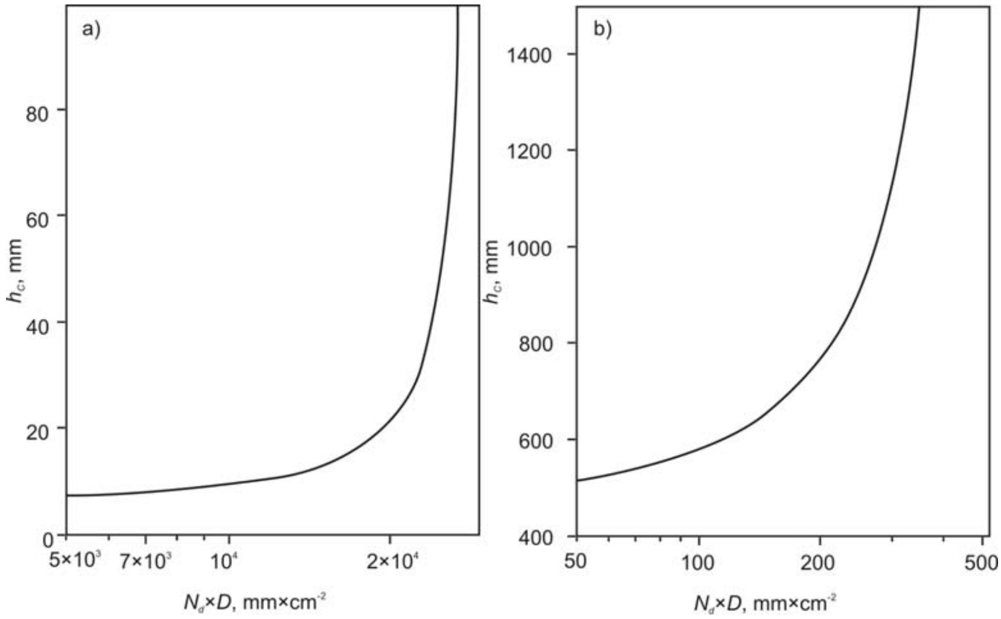

Fig. 4. Dependences of the critical thickness for dislocation removal from the epitaxial layer upon the characteristic sample size and the dislocation density in the case of doping by: a) Bi, b) Pb

Figure 4 shows how the critical thickness associated with dislocation removal (from the inner epitaxial layer to the boundary) depends on the product of two factors: the characteristic size of the sample and the density dislocation in the sample. Bi and Pb concentrations in Fig. 4 have been accepted at the highest possible level of real achievable values being 5×10^{18} cm^{-3} [18] and 4×10^{17} cm^{-3} [19] for Bi and Pb, respectively.

As follows from Fig. 4, starting from certain values of the dislocation density in the substrate and the sample size, the critical thickness of the epitaxial layer that enables removal of threading dislocations to the edge of the epitaxial layer increases dramatically. The increase in the thickness of epitaxial layers requires higher initial growth temperatures, which then leads to other defects such as point defects and impurities. It degrades the influence of the decrease of dislocation density on the electrophysical parameters of material. In this respect, the effective reduction of the threading dislocation density in the epitaxial layer at isovalent doping is only possible at certain values of A that depends on the product of DN_d.

Using the results shown in Fig. 4, the following expressions can be obtained in the case of Bi (Eq. (14)) and Pb (Eq. (15)) doping:

$$D \le \frac{2\times10^4}{N_d} \tag{14}$$

$$D \le \frac{300}{N_d} \tag{15}$$

In Equations (14) and (15) D is expressed in millimetres and N_d in cm^{-2}.

A relatively small solubility of Pb in solid GaAs leads to a very thick epitaxial layer (hundreds of micrometers, Fig. 4b) when dislocations start to glide. That is why Pb is not an effective dopant for removing dislocations from the epitaxial layer to the edge of the structure.

The considered approach can be used for estimating the effectiveness of removing dislocations from the epitaxial layer at use compared with other methods of epitaxy. Molecular beam epitaxy (MBE) and vapour phase epitaxy (VPE) methods provide higher concentrations of isovalent doping of the epitaxial layer than LPE. Additional use of mesastructures makes it possible to decrease the value h_c considerably, up to the conventional epitaxial layer thicknesses obtained by MBE and VPE.

4. Conclusions

In this paper, an exact analytical solution is given for the critical thickness, h_c, of the epitaxial layer that permits the removal of threading dislocations from the interior of the epitaxial layer to its edge. It makes it possible to analyse the dependence of h_c on the geometrical and mechanical parameters of substrates. The critical thickness of the epitaxial layer permitting the motion of threading dislocations can be obtained by substituting $L = 0$ in Eq. (10).

The product DN_d has been shown to be the critical parameter determining the effectiveness of the dislocation removal from the epitaxial layer. Because of the absence of extreme points in the dependence $h_c(DN_d)$, there is no optimal combination of D and N_d which can provide the most effective removal of dislocations from thin epitaxial layers. With increasing DN_d, h_c increases monotonically.

The analysis of the dependence of the critical thickness of the epitaxial layer on the product DN_d makes it possible to quantify the isovalent doping for introducing strains in the epitaxial layers to reduce the threading dislocation density.

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