Calculation of thermoelastic stresses in ribbon gallium oxide crystals grown from a melt by the Stepanov method (EFG) in various crystallographic orientations.

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In this work, we investigated the effect of anisotropy on the distribution of thermoelastic stresses in thin crystalline gallium oxide plates. Approximate formulas for the components of the stress tensor are given, obtained using the asymptotic integration of the thermoelasticity equations taking into account rectilinear anisotropy of a general form. A comparison of stress values for two growth directions was carried out. It is shown that choosing the orientation of the growth direction makes it possible to control the magnitude and distribution of thermoelastic stresses that arise in gallium oxide crystals when they are grown from a melt.

Keywords: thermoelastic stresses, asymptotic method, anisotropy of thermal and elastic properties.

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Introduction

Gallium oxide (β-Ga_2O_3) is an ultra-wide bandgap semiconductor (> 4.4 eV) with a high breakdown voltage (> 8 MV/cm). It is actively being studied as a promising new generation power semiconductor [1,2]. The bulk single-crystals of gallium oxide in the form of cylinder boules are grown from melt by different methods. The largest number of studies and publications are devoted to Czochralski method, where a crystal is pulled out from the melt in the iridium crucible. Despite a number of technological difficulties, crystals in the form of cylinders up to 50 mm in diameter have been grown to date [3]. However, plate like crystals are required for the most applications. Therefore, it is required to cut the grown boules followed by further grinding and final polishing of the fabricated plates. The idea of growing crystals of a given profile, in particular, plates of a given size, has gained some interest. The edge-defined film-fed growth (EFG) (Stepanov method) is the only method that makes it possible to grow crystals in the form of plates. In this method, a crystal is grown from a melt in a crucible into which a shaping device is placed. In the simplest case, this is a plate with capillary channels through which the melt rises to the upper edges of the plate, which determine the shape and size of the crystal [4,5]. This method has been successfully used to produce gallium oxide crystals (β-Ga_2O_3). Unlike Czochralski method, here the crucible can be covered with a lid, which reduces decomposition and evaporation of the melt. Due to this, as well as the possibility of wafer growth at a higher rate, crystals of good quality are obtained. It is by this method that substrates up to 6 inches in size are currently produced (Tamura corp, Novel Crystal Technology Inc.) [6].

For the first time, the growth of β-Ga_2O_3 plate 2 inch wide was demonstrated by Shimamura [7]. High-quality single-crystal two-inch plates were grown by Hideo Aida [8]. In Akito Kuramata study they used EFG method to grow crystals with a size of up to 4 inches [9]. Huili Tang paper describes the improved EFG technology that allowed to grow large-size single crystals of β-Ga_2O_3 without the sub-grain boundaries and cracks [10]. Yuzhe Bu studied the formation of twins in β-Ga_2O_3 crystals and grew the crystals with orientation (100) using EFG method [11]. In the study performed by Chengcheng Lea a numerical modeling was made for the thermal field in the gallium oxide crystals growth zone in order to find optimal growing conditions [12]. Woon-Hyeon Jeong studied the impact of active after-heater on the growth of gallium oxide single crystals by EFG method [13].

However, despite all efforts to improve the growth process, many questions still remain unclear. For example, it has been experimentally found that the best crystallographic direction for growing bulk crystals of gallium oxide is [010]. Plate-shaped crystals are grown in the same direction, and the plate plane varies from $(\bar{2}01)$ to (100) according to different authors.

It is well known that the thermoelastic stresses that arise in grown crystals due to the nonlinearity of temperature fields largely determine the degree of their structural perfection. They can lead to plastic deformation associated with the formation and movement of dislocations, formation of small-angle boundaries, blocky, and possibly twin structures. It has also been established that the anisotropy of thermophysical and elastic properties significantly impacts the magnitude and distribution of stresses, which provides a possibility of controlling the degree of their structural perfection by choosing the crystallographic orientation of the crystals [14,15].

However, for gallium oxide crystals, no detailed study of the influence of crystallographic orientation, as well as anisotropy of properties on growth, thermoelastic stresses and crystal quality has been carried out. In paper [16] it was shown that for cylindrical crystals of gallium oxide, the growth orientation significantly affects the distribution of thermoelastic stresses due to the strong anisotropy of thermal and elastic properties.

In this paper, the effect of anisotropy of thermal and elastic properties of gallium oxide on the magnitude and distribution of thermal stresses in ribbon-shaped crystals grown from a melt by Stepanov method (EFG) is investigated. Approximate asymptotic formulas describing stress fields in thin, narrow plates were used for calculations. These formulae are obtained by asymptotic integration of thermal elasticity equations in the presence of general rectilinear anisotropy [17].

1. Approximate Formulae for Thermoelastic Stresses

The thermal conductivity, thermal expansion and elastic stiffness coefficients of gallium oxide measured for the standard coordinate system ($\bar{x}_3$ axis coincides with the crystallographic orientation [001], and $\bar{x}_1$ axis — coincides with [100]) were taken from the study [18]. Here, we present only thermal conductivity coefficients, since thermal expansion and elastic stiffness coefficients were given in paper [16]. Thus, gallium oxide thermal conductivity coefficients extrapolated to a temperature of 2000 K (dimensions $\mathrm{Wm^{-1}K^{-1}}$): $\bar{\lambda}_{11} = 1.23$, $\bar{\lambda}_{12} = \bar{\lambda}_{21} = 0$, $\bar{\lambda}_{13} = \bar{\lambda}_{31} = 0.38$, $\bar{\lambda}_{22} = 2.11$, $\bar{\lambda}_{23} = \bar{\lambda}_{32} = 0$, $\bar{\lambda}_{33} = 1.63$. The dimensional values are indicated by a line at the top.

Let us consider a straight crystalline plate of length l with a rectangular cross-section $\Omega = [-b, b] \times [-h, h]$ ($2b$ is the width of the plate, $2h$ is its thickness). We'll use Cartesian coordinate system $(\bar{x}_1, \bar{x}_2, \bar{x}_3)$. The $\bar{x}_1$ axis is orthogonal to the plane of the plate, the $\bar{x}_2$ and $\bar{x}_3$ axes lie in the median plane, and the $\bar{x}_3$ axis coincides with the growth direction. Let us move on to the dimensionless coordinates as follows:$\bar{x}_1 = hx_1$, $\bar{x}_2 = bx_2$, $\bar{x}_3 = lx_3$. Let us proceed to the dimensionless coefficients of thermal conductivity, thermal expansion and elastic compliance by normalizing to the corresponding invariants: $\bar{\lambda}_{00} = 1.657$ ($\mathrm{Wm^{-1}K^{-1}}$); $\bar{\alpha}_{00} = 7.17 \cdot 10^{-6}$ ($\mathrm{K^{-1}}$); $\bar{s}_{00} = 0.051 \cdot 10^{-10}$ ($\mathrm{m^2/N}$). By assuming the small values of parameters $\delta = h/b$, $\varepsilon = b/l$ and weak heat exchange on the edges $x_1 = \pm 1$ let's find the solution of the stationary thermoelastic problem. Using the method of asymptotic integration of the thermoelastic equations [19] we obtain with an accuracy of terms of order δ^0, ε^2 the formulae for the temperature and components of the thermoelastic stress tensor in a crystalline plate:

$$\bar{T}|_{\delta=0} = \Bigg\{ T_0(x_3) + \left[T_1(x_3) + \mu x_2 \frac{dT_0(x_3)}{dx_3} \right] \varepsilon + \left[T_2(x_3) + \mu x_2 \frac{dT_1(x_3)}{dx_3} + \frac{1}{2}\mu^2 \left(x_2^2 - \frac{1}{3} \right) \times \frac{d^2 T_0(x_3)}{dx_3^2} \right] \varepsilon^2 \Bigg\} \bar{T}_{00},$$

$$\bar{\sigma}_{33}(x_2, x_3)|_{\delta=0} = -\frac{1}{6} H (3x_2^2 - 1) \bar{\Delta} \frac{d^2 T_0(x_3)}{dx_3^2} \varepsilon^2,$$

$$\bar{\sigma}_{23}(x_2, x_3)|_{\delta=0} = \frac{1}{6} H (x_2^2 - 1) x_2 \bar{\Delta} \frac{d^3 T_0(x_3)}{dx_3^3} \varepsilon^3,$$

$$\bar{\sigma}_{22}(x_2, x_3)|_{\delta=0} = -\frac{1}{24} H (x_2^2 - 1)^2 \bar{\Delta} \frac{d^4 T_0(x_3)}{dx_3^4} \varepsilon^4,$$

where

$$H = \frac{1}{s_{33}} [\alpha_{22} + \mu(\alpha_{33}\mu - 2\alpha_{23})], \quad \mu = \frac{\lambda_{12}\lambda_{13} - \lambda_{11}\lambda_{23}}{\lambda_{11}\lambda_{22} - \lambda_{12}^2}.$$

Here, $T_0(x_3)$, $T_1(x_3)$, $T_2(x_3)$ — are the first expansion terms for a cross-section average dimensionless temperature in powers of the small parameter ε; d^2T_0/dx_3^2 — the dimensionless second derivative of temperature along the direction of plate growth; $\bar{T}_{00}$ — melting point of gallium oxide (2080 K). The temperature is normalized to the melting point ($\bar{T} = T\bar{T}_{00}$). In formulae for components of the thermoelastic stress tensor $\bar{\Delta} = \bar{\alpha}_{00}\bar{T}_{00}/\bar{s}_{00}$ is a normalizing multiplier that provides a transition from dimensionless to dimensional components of the thermoelastic stress tensor.

2. Thermoelastic stresses calculation results

The case of growing β-GaO_3 crystal as a rectangular plate 0.1 m long, 0.02 m wide and 0.002 m thick was analyzed. Since there is no experimental data on the temperature field of the grown crystal, for calculations we used a model temperature distribution along the axis of growth with constant curvature $d^2\bar{T}_0/d\bar{x}_3^2 = -5 \cdot 10^4\,\mathrm{K/m^2}$. Two crystallographic orientations of the growing plate were considered. First: growth direction along [010], normal to the wider side along [100], and then rotation around the growth axis (Fig. 1, a). This orientation is most often used in practice when growing crystals of β-GaO_3. Second orientation — standard system with the growth direction [001] (Fig. 1, b). The analysis of the formulae obtained for the components of the thermoelastic stress tensor shows that the maximum stress values are observed for the component σ_{33}. It should be noted that the above stress formulae are valid in the middle part of the ribbon. In the face ends also σ_{23}, σ_{22} components are acting, with the values comparable to σ_{33}. Fig. 2 illustrates the distribution of σ_{33} component across the

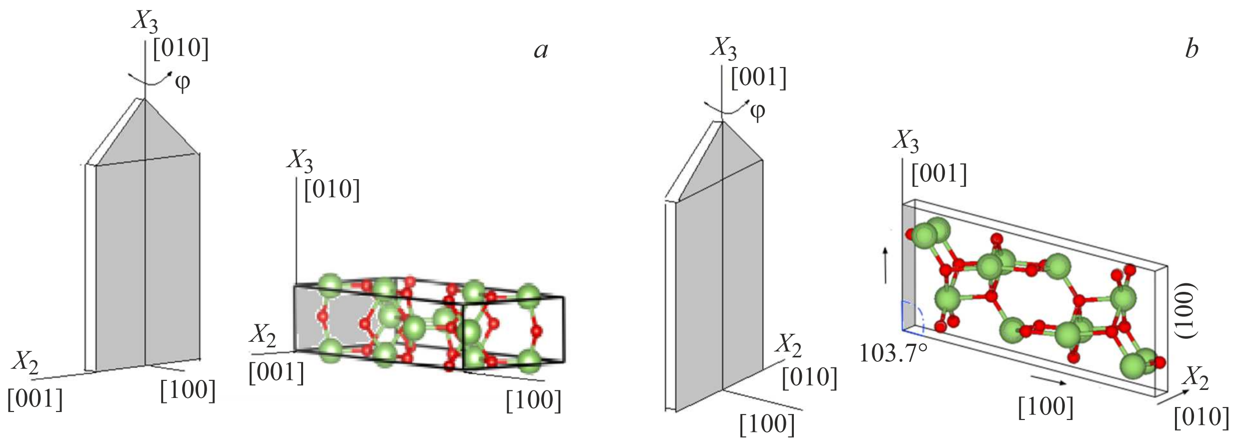

Figure 1. Patterns of two crystal-lattice orientations of the grown plate: in direction [010] (*a*) and in direction [001] (*b*). Lattice cells β-Ga_2O_3 are shown on the right of them.

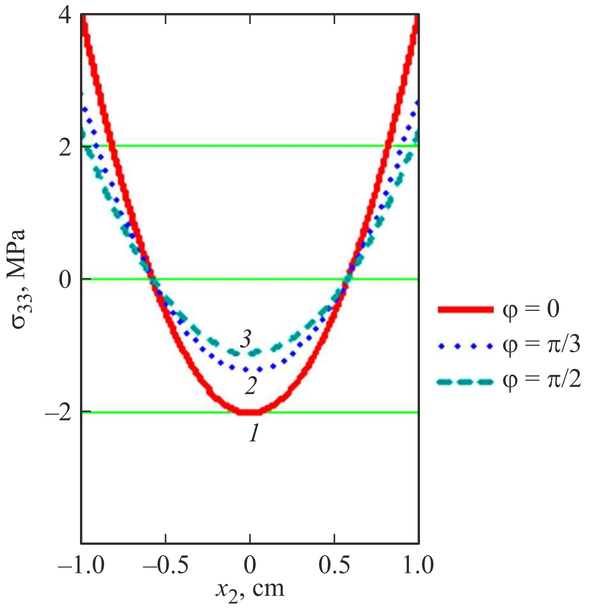

Figure 2. Distribution of stress σ_{33} over the plate width when crystals are grown in [010] direction. Curve *1* — initial position $\varphi = 0$, curve *2* — rotation around [010] by an angle $\varphi = \pi/3$, curve *3* — rotation by $\varphi = \pi/2$.

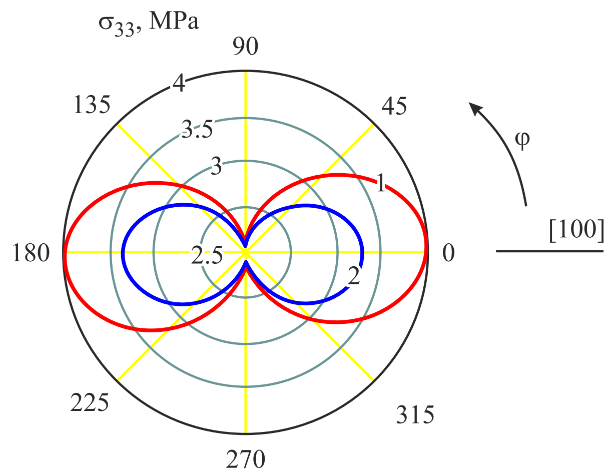

Figure 3. Stress σ_{33} versus rotation angle φ in polar coordinates for the two cases of plate growth: in direction [010] — curve *1* and in direction [001] — curve *2*.

ribbon width. In accordance with the formula given above, σ_{33} varies in width of the ribbon along a parabola. Fig. 3 demonstrates the results of calculation of σ_{33} component when the crystal-lattice orientation is rotated at φ around the growth direction [010] (curve *1*) and around [001] (curve *2*). The maximum stress values σ_{33} are fixed for the direction [010] at the normal to the plane directed along [100], and the minimum — at the normal to the plane directed along [001]. Therefore, from the point of view of minimizing thermoelastic stresses, this orientation can be recommended for crystals growing.

The lower stress level during growth in [001] direction turned out to be somewhat unexpected for the similar nature of the angular dependence. However, this is not confirmed in the experiment. Other factors may also influence the growth and formation of the defective structure. The calculations show a strong influence (up to 50%) of anisotropy of the gallium oxide ribbon crystal properties and the orientation of the growth direction on thermoelastic stresses.

Conclusion

A comparison of stress values for two growing directions was carried out. It is shown that by accounting the anisotropy of elastic properties and thermal expansion, as well as by selecting the proper orientation of the gallium oxide ribbon-like crystals growth relative to the crystallographic axes, it is possible to control the magnitude and distribution of thermoelastic stresses arising in them during growth, and therefore the degree of its structural perfection.

Conflict of interest

The authors declare that they have no conflict of interest.

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