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Theoretical study of the formation of deformation twins in GaAs crystals grown by the vertical gradient freeze method

A. N. GULLUOGLU
Department of Material Science and Engineering, Marmara University, Goztepe, Istanbul, Turkey

XINAI ZHU, C. T. TSAI
Department of Mechanical Engineering, Florida Atlantic University, Boca Raton, FL 33431, USA
E-mail: tsaict@fau.edu

The objective of this paper is to predict the twin formation in the Gallium Arsenide (GaAs) crystals grown by vertical gradient freeze (VGF) method at different growth parameters. The deformation twins are formed in the GaAs crystal during its growth processes from the melt. The thermal stresses generated by the temperature profile during the crystal growth can be the primary cause of deformation twin formation. Temperature gradients are depend on the geometrical and physical crystal growth parameters, such as crystal diameter and imposed temperature gradients on the surface of the solidifying crystal in VGF. A quantitative thermal stress model is developed here for predicting the twin formation in GaAs grown by VGF at different growth parameters. This investigation is expected to further the understanding of twin formation. This understanding will provide valuable information to crystal growers to study the influence of growth parameters on twin formation for growing low defect GaAs crystal.

1. Introduction

GaAs single crystals are becoming more important and finding wider applications in semiconductor device technology. Due to its high mobility, saturated drift velocity and the ability to produce semi-insulating substrates, GaAs semiconducting devices have superior performance in comparison to silicon. However, the presence of defects (twins and dislocations) in GaAs crystals are much more than that in Silicon crystals. It is well known that the crystal defects in these materials adversely affect the lifetime and performance of these devices [1]. For example Weiss *et al.* [2] have observed the degradation of current–voltage (I–V) and capacitance–voltage (C–V) characteristics of photodiodes and MIS capacitors. These persuasive results suggest that commercial viability of high-speed electronic and photonic devices and circuits strongly depends on the availability of low defect GaAs crystals.

Defects are created by thermal stresses in the crystals, which is result of temperature gradients developed during the growth process. The gradients result from the heater and insulator geometry of the crystal growth process, and physical parameters. Methods used to reduce temperature gradients in the liquid encapsulated Czochralski (LEC) include the use of multiple heaters, heat shields, gas baffles [3]. The temperature gradients in the VGF [4], are attained via an empirically optimized combination of insulation, heat shields and the spatial distribution of heat input. Since the VGF method achieve a low temperature gradient, it is a novel process to grow III-V semiconductor crystals with large diameter and low dislocation density and twins.

Twinning in the diamond cubic and zinc blende semiconductor crystals is represented by a 60 rotation about normal direction of the {111} twinning plane [5]. It has been demonstrated by Billig [6] that such twinning commonly occurred on {111} "edge" facets on the crystal-melt interface in the vicinity of the three phase boundary (TPB). Numerous factors (i.e., the seed orientation, conical growth angle, interface shape, an In-rich melt, temperature gradient, and temperature fluctuations) affecting the formation of twinning have been found from practical experience [5]. Hurle [7] has proposed a model to explain the possible cause of the twinning phenomenon. He found that twinning occurs when three conditions are simultaneously satisfied [5]. The three conditions are (1) An edge facet is attached to the TPB, (2) The external surface of the growing crystal is so oriented that its extension by the formation of a twinning nucleus produces a segment of ⟨111⟩ oriented surface and the meniscus contact angle is such that equilibrium can exist at the TPB, (3) The supercooling on the edge facet exceeds a critical value. The three conditions in Hurle's model affect the shear stress on the twinning plane and could enhance the incidence of deformation twins if high shear stresses acting on the twinning plane are generated. Friedel [8] found that the theoretical shear stresses necessary for a homogenous nucleation of a deformation twin in a crystal lie between 1/30 to 1/500 μ of the theoretical elastic limits, where μ is the shear modulus. For GaAs, the shear modulus is about 2.75×10^{10} Pa at melting point and 1/500 μ is about 55 Mpa [9]. This is a strong evidence for the belief that deformation twins are nucleated heterogeneously in the regions of high shear stress concentration in the crystal. It is therefore probable that the slip process must be impeded by barriers, such as subgrain boundaries, grain boundaries, other dislocations, and impurities, which prevent the motion of dislocation in certain regions. These regions may lower the magnitude of stress needed to nucleate the deformation twins [10].

Deformation twins are formed when the resolved shear (RSS) stresses acting along the twinning direction on the twinning plane exceeds the critical resoled shear stress (CRSS) for twin formation. In practical, the CRSS could be smaller than the theoretical shear stresses necessary for homogenous nucleation of a deformation twin. But, because the localized stress fields can be formed in different ways, depending on the geometry and orientation of the specimen, it is probable there can be no universal CRSS for the development of twins.

The motion of partial dislocations can create deformation twins. If a slip dislocation with Burgers vector b, splits up in to, such as, a Shockley partial dislocation with a Burgers vector (a/6) $[1\bar{2}1]$ moves across each (111) closed packed plane contained in a section of an zinc blende structure as shown in Fig. 1, it changes the stacking squence from Aa Bb Cc to Bb Cc Aa in this section of the crystal. It can be seen from Fig. 1. that partial dislocations are in the act of changing the stacking squence. The resulting arrangement constitutes an intrinsic stacking fault, which is one double-layer thick twin [11]. It can be seen from Fig. 1b that an individual partial dislocation is associated with a stacking fault, and only one of the partials is connected to a fault. This is the dislocation that lies on the boundary between the twinned and untwinned regions. Successively faulting each plane of atoms in a crystal produces a new perfect crystal. Therefore, except at the boundary, the stacking faults have cancelled one another out. The orientation of the new crystal, the twin, is that of a mirror image of the original crystal reflected in the boundary plane. Any one of partials that creates a twinned region is called twinning dislocation. In this model, twins are considered composed of long straight parallel partial dislocations on successive {111} planes, and are created under the action of stress concentration.

Formation of deformation twins depends strongly on the temperature gradient present during crystal growth. Deformation twins are formed when RSS in the twinning systems exceeds the CRSS for the crystal. Even though the experimental data for CRSS of GaAs are not available at present, the development of a numerical model for predicting twin formation is valuable by assuming a CRSS to provide comparative study of twin formation during crystal growth. This comparative study will provide valuable information to improve

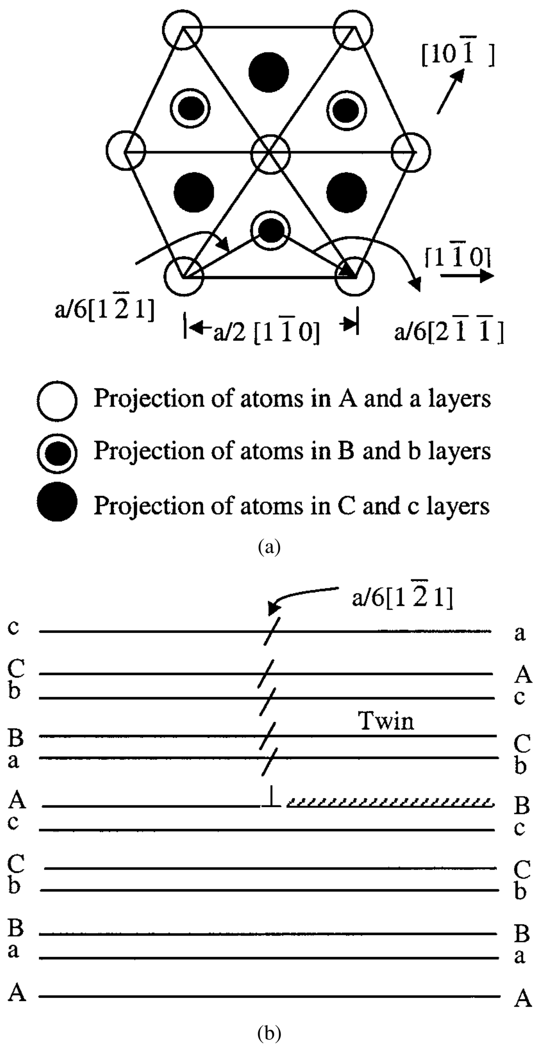


Figure 1 (a) The (111) plane of a diamond cubic structure. (b) Illustration of a twin in the diamond cubic and zinc blende structures.

the understanding of the twin formation in GaAs crystals grown from the melt. Furthermore, it can be employed for optimizing the growth configurations and parameters for growing GaAs crystals with the minimum twin formation. If one can obtain the CRSS from the experimental measurements, the data can be directly employed to the developed model and more accurate results can be obtained. In the following section, the basic simulation procedure for studying the twin growth is summarized. Results of numerical simulations are presented and analyzed in Section 3. Finally, the last section presents a discussion of the numerical results.

2. Simulation model of twin formation

In the crystal growth processing which is shown in Fig. 2a, a cylindrical ingot with a near planar solid-liquid interface at $z = 0$ is solidified from the melt at rate p by the VGF method [4]. Since the numerical modeling of heat and mass transport in VGF growth process is not the objective of this study, we use the analytical solution of temperature distribution first given by Jordan *et al.* [12]. In the calculation of temperature distribution which are used to model the residual stress state and twin formation in the crystals, the partial

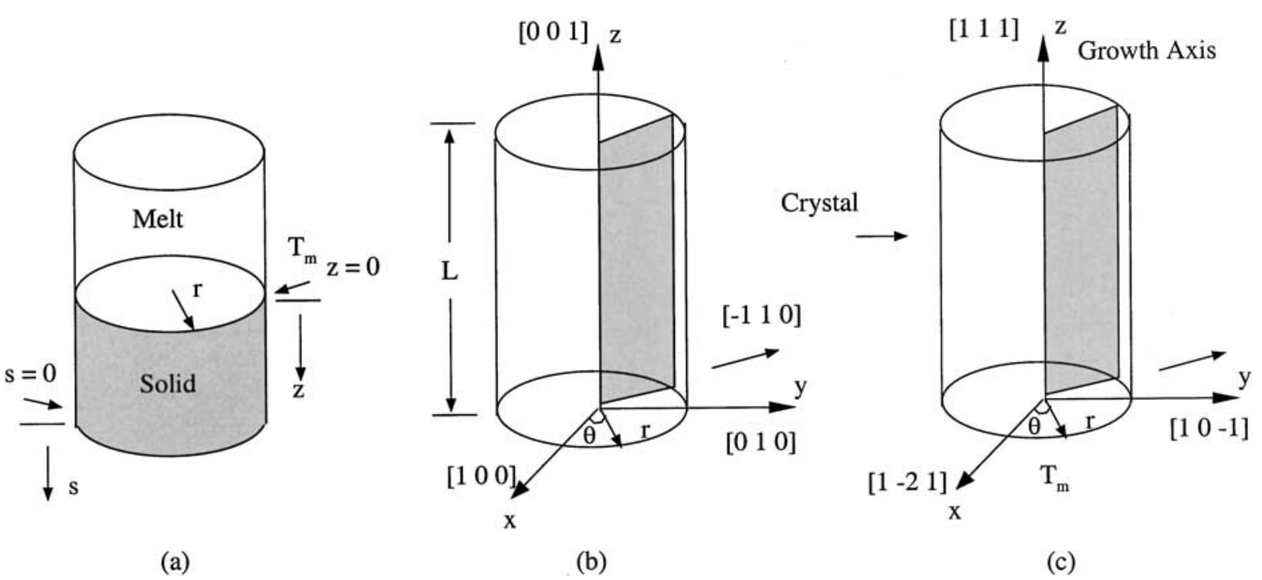


Figure 2 Coordinate system of the crystal pulling, (a) stationary, s, and moving, z, systems, (b) the [001] and (c) the [111] direction during crystal growth, where T_m is the melting point along the solid-melt interface of the crystal.

differential equation in cylindrical coordinate system with cylindrical symmetry in boundary conditions for heat conduction [12, 13] is solved,

$$\frac{\partial T}{\partial t} = \kappa\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial s^2}\right), \qquad (1)$$

where, κ is thermal diffusivity, and $s = 0$ is at the bottom of the crucible in fixed coordinate system. Through the introduction of a moving coordinate system [12, 14], $z = s + \mathrm{pt}$ at solid-liquid interface, Equation 1 becomes,

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} = \frac{p}{\kappa}\frac{\partial T}{\partial z}. \qquad (2)$$

Temperature distribution is calculated in crystalline solid by solving Equation 2 under the assumptions [9]: (1) a cylindrical crystal with a radius of r_o, and length of L growing in time t at a constant rate, p, with a planar solid-melt interface at a temperature T_m; (2) solidification is controlled by the imposed temperature gradient v at the crucible; and (3) base of the crucible is insulated so that a quasi-steady-state temperature distribution is attained. Even though a nonplanar solid-melt interface is grown by VGF method at practical growth rates for given thermal properties of the crucible and furnace, it has been experimentally found that the isotherm of the melting point in VGF grown InP crystals is nearly planar [11]. The temperature distribution in the crystal is given by [14]

$$T = T_m + 2e^{p_1\frac{\psi}{2}} \sum_{n=1}^{\infty} \frac{I_0(\overline{\alpha}_n\rho)(\sin\beta_n)\psi \mathrm{G}}{I_0(\overline{\alpha}_n\rho_0)\left[1 + \frac{(\sin^2\beta_n)p_1}{2\beta_n^2}\right]}, \qquad (3)$$

where, $\psi = z/L + 1$, $\rho = r/L$, $\rho_0 = r_0/L$, $p_1 = pL/\kappa$, and

$$G = \mathrm{v}L\frac{e^{\frac{-p_1}{2}}(\sin\beta_n)\overline{\alpha}_n^2 + p_1\beta_n}{\overline{\alpha}_n^4} \qquad (4)$$

In Equation 1, I_0 is the modified Bessel functions of first kind, order zero, with eigenvalues

$$\beta_n \cot\beta_n + p_1 = 0; \qquad \overline{\alpha}_n^2 = \beta_n^2 + \frac{p_1^2}{4}. \qquad (5)$$

for determining the α_n [15]. Although several simplifying assumptions are made in the analytical temperature calculation, this temperature distribution adequately approximates a typical growth temperature distribution for our parametric study of twin formation in VGF grown GaAs crystals. Material parameters in for GaAs material, T_m is 1511 K and κ is 4×10^{-6} m^2/s.

The temperature gradients induce a thermal stress field in the growing crystal because of spatially inhomogeneous thermal contraction. The thermoelastic stresses in VGF grown crystal are calculated from a two-dimensional finite element analysis. In the model, the growing crystal ingot is assumed to be an axisymmetrical solid (Fig. 2). If u and w are displacement components in the r and z directions, respectively, then the strain components in the cylindrical coordinates are

$$\varepsilon_{rr} = \frac{\partial u}{\partial r}, \quad \varepsilon_{\theta\theta} = \frac{u}{r}, \quad \varepsilon_{zz} = \frac{\partial w}{\partial z},$$
$$\varepsilon_{rz} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial r}\right). \qquad (6)$$

By assuming GaAs crystal as an elastically isotropic material, the stress-strain relations are

$$
\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{rz} \end{Bmatrix} = \frac{E}{(1+\nu)(1-2\nu)}
\times \begin{bmatrix} (1-\nu) & \nu & \nu & 0 \\ \nu & -\nu & \nu & 0 \\ \nu & \nu & (1-\nu) & 0 \\ 0 & 0 & 0 & \dfrac{(1-2\nu)}{\nu} \end{bmatrix}
\times \begin{Bmatrix} \varepsilon_{rr} - \alpha\Delta T \\ \varepsilon_{\theta\theta} - \alpha\Delta T \\ \varepsilon_{zz} - \alpha\Delta T \\ \varepsilon_{rz} \end{Bmatrix}. \tag{7}
$$

where, E, ν and α are Young's modulus, Poisson's ratio, and thermal expansion coefficient of GaAs, ΔT is the temperature change, subscripts rr, $\theta\theta$ and zz refer to the r, θ and z coordinate system of Fig. 2. Based on Equations 6–7 and the principle of virtual work, a finite element equation for the thermal-elastic problem of quasi-steady-state crystal growth in terms of displacement fields is given as [16].

$$
[K_\mathrm{s}(T)]\{U\} = \{F_\mathrm{T}\} + \{F_\sigma\} + \{F_\mathrm{b}\} = \{F\}, \tag{8}
$$

where $[K_\mathrm{s}(T)]$ is the stiffness matrix, which is a function of temperature; U represents the nodal displacements u and w; and the terms on the right hand side are thermal loading (F_T), surface tractions (F_σ) and body forces (F_b), respectively.

The thermal stress calculation are performed in cylindrical coordinate system in which z axis is assigned to be a growth axis in this simulations, either [001] or [111] as shown in Fig. 2. In the simulations, x//[100], y//[010] and z//[001] are chosen in the case of crystal growth direction of [001], and if the growth direction is [111], x//[1$\bar{2}$1], y//[10$\bar{1}$] and z//[111] are selected. The cylindrical stress components σ_{rr}, $\sigma_{\theta\theta}$, σ_{zz} and σ_{rz} are transformed into a Cartesian coordinate system by use of the stress transformation tensor, $\sigma_{ij} = \sigma_{kl} l_{ik} l_{jl}$, where l_{ik} and l_{jl} are direction cosines, $(i, j, k, l = 1, 2, 3)$, σ_{ij} and σ_{kl} are stress tensor in Cartesian and cylindrical coordinate system, respectively.

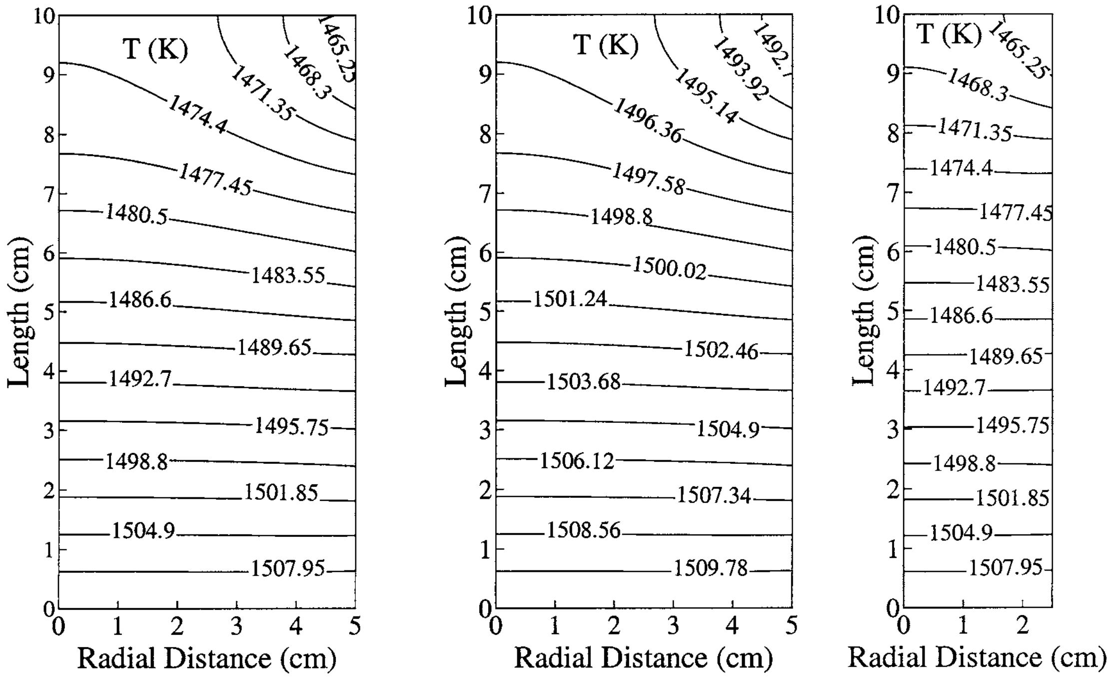
GaAs crystals have crystal structure of zinc blende. The twining plane in the zinc blende structure is {111} and twinning directions are ⟨112⟩. Twelve twinning systems can be considered in the present crystal system [17]. Formation of deformation twins in semiconductors depends on the magnitude and directions of the shear stresses on twinning systems. Necessary condition for twinning is that the shear stress resolved on the twinning plane and in the twinning direction shall reach the CRSS which is characteristic of the crystal. A local coordinate system (x', y', z') is defined for calculation of RSS in each twinning system in which twining direction is along x', y' is normal to the twinning plane, and z' is parallel to cross product of x' and y' vectors. The global stress tensor in Cartesian coordinate system is transformed into the local coordinate system of twins by use of the stress transformation tensor, $\sigma_{i'j'} = \sigma_{kl} l_{i'k} l_{j'l}$ where $\sigma_{i'j'}$ and σ_{kl} are stress tensor in local and global coordinate systems, respectively. The RSS acting on the 12 twinning systems are then calculated using this model.

3. Results and discussions

The GaAs ingots grown by VGF is presented as an example for investigating effect of growth parameters on twin formation in the crystal using the developed numerical model. The three different temperature profiles (melting point of GaAs, 1511 K) for the VGF grown GaAs crystals after about 25 hours of growth (10 cm long crystal) are calculated by solving Equation 3. Fig. 3 shows the three calculated temperature distribution for 5 cm radius GaAs crystal grown by VGF at (a) $v = -5$ K/cm, at (b) $v = -2$ K/cm, and for (c) 2.5 cm radius GaAs crystal grown by VGF at $v = -5$ K/cm. In these three cases (a)–(c), the length of crystal is about 10 cm and growth rate is 1.16×10^{-4} cm/s.

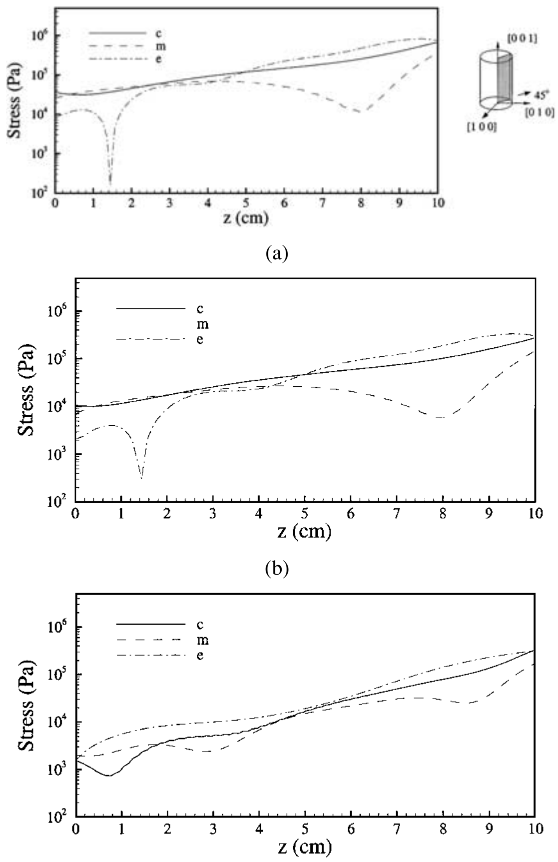
Twinning depends on the magnitude and direction of RSS on twinning systems. For comparison purposes, temperature distributions shown in Fig. 3 are employed to calculate RSS in all twinning systems of crystal for different growth parameters and directions. Effect of crystal growth direction on twin formation has been investigated for the [001] and [111] pulling directions. The major factors influencing the deformation twin formation are the resulting thermoelastic stresses induced by the temperature gradient during the growth of crystal. In order to understand the effect of growth parameters on twin formation, RSS in each twinning system along the growth direction, near the center ($r = 0.1$, and 0.05 cm), the middle ($r = 2.5$, and 1.25 cm), and the edge ($r = 4.8$, and 2.4 cm), of 5 and 2.5 cm radius wafers have been calculated for three different cases separately. The calculated results show that RSS varies greatly with twinning systems. The ($\bar{1}1\bar{1}$)[$\bar{2}\bar{1}1$] twinning system has one of the highest RSS among twinning systems for crystals grown along [001] and [111] directions. In this high RSS twinning system, RSS along the three column positions on (1–1 0) plane for GaAs crystal grown for cases (a)–(c) are shown in Fig. 4. It can be seen from Fig. 4a–c that RSS near the edge and center of the wafer are much greater than that near the midway of the wafer along the [001] growth direction, even though the growth parameters are different. Fig. 5 shows the RSS for ($\bar{1}1\bar{1}$)[$\bar{2}\bar{1}1$] twinning system along the three column positions on the 45° crystal plane for crystal grown in [111] growth direction for cases (a)–(c). Figs 4 and 5 show that even though the crystal growth parameters are different, RSS increases along the length of the VGF grown crystal, and the maximum RSS are always located near the edge of the wafer. Figs 4 and 5 demonstrate that RSS near the edge of the wafer for growth direction of [111] are greater than that for the growth direction of [001].

Calculated RSS in the {111}, ⟨11$\bar{2}$⟩ twinning systems for GaAs crystal grown at different growth parameters



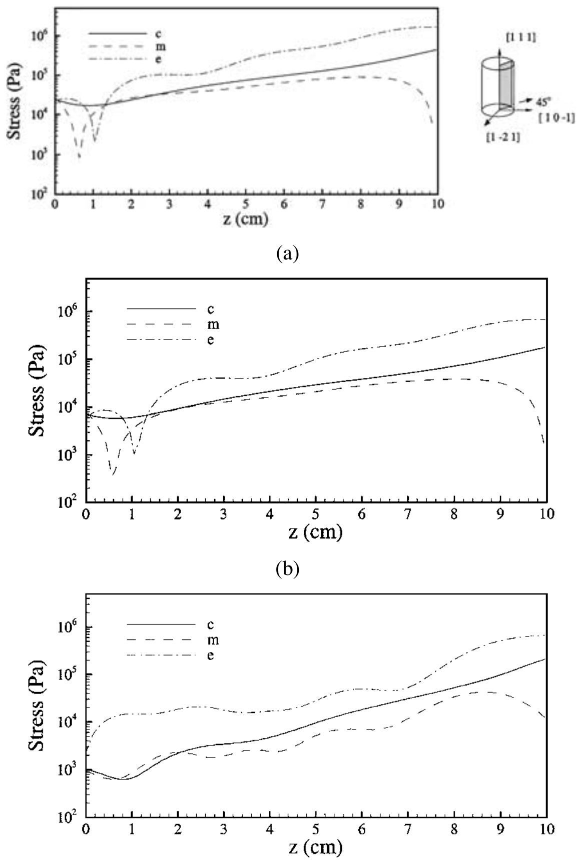
(a) (b) (c)

Figure 3 Temperature distribution for 5 cm radius GaAs crystal grown at (a) $v = -5$ K/cm, (b) $v = -2$ K/cm, and for (c) 2.5 cm radius GaAs crystal grown at $v = -5$ K/cm.



(a) (b) (c)

Figure 4 The RSS on $(1\bar{1}0)$ plane along the [001] growth direction near the center, the middle, and the edge of the wafer for $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$ twinning system for GaAs crystal grown by VGF for cases (a)–(c).



(a) (b) (c)

Figure 5 The RSS on the 45° plane along the [111] growth direction near the center, the middle, and the edge of the wafer for $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$ twinning system for GaAs crystal grown by VGF for cases (a)–(c).

(Figs 4–5) show that the maximum RSS are always located near the top of the crystal. Therefore, RSS contour line pattern near the top of the crystal on the (001) GaAs wafer grown at $r = 5$ cm and $v = -5$ K/cm (case a) are studied for each twinning system along the growth direction of [001] and shown in Fig. 6 for twinning systems (a) $(\bar{1}1\bar{1})[\bar{2}11]$, (b) $(\bar{1}1\bar{1})[\bar{1}12]$ and (c) $(1\bar{1}\bar{1})[12\bar{1}]$. The RSS contour lines for the 12 twinning systems

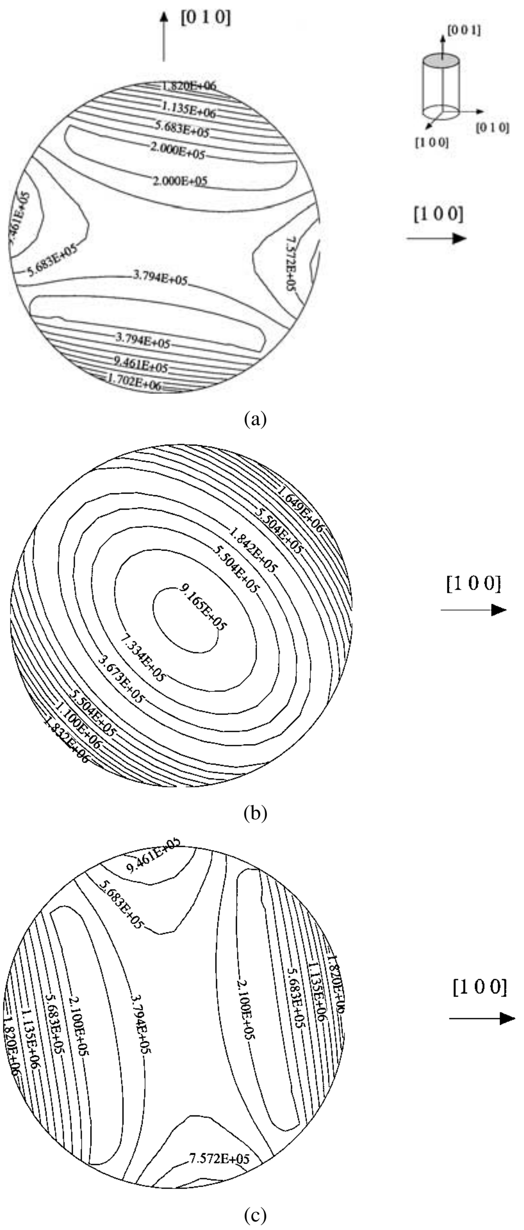


Figure 6 The RSS distribution near the top of the crystal on the (001) GaAs wafer grown, at $r = 5$ cm and $v = -5$ K/cm along [001] growth direction for (a) $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$, (b) $(\bar{1}1\bar{1})[\bar{1}12]$ and (c) $(1\bar{1}\bar{1})[12\bar{1}]$ twinning systems. The numbers on the contours are in Pa.

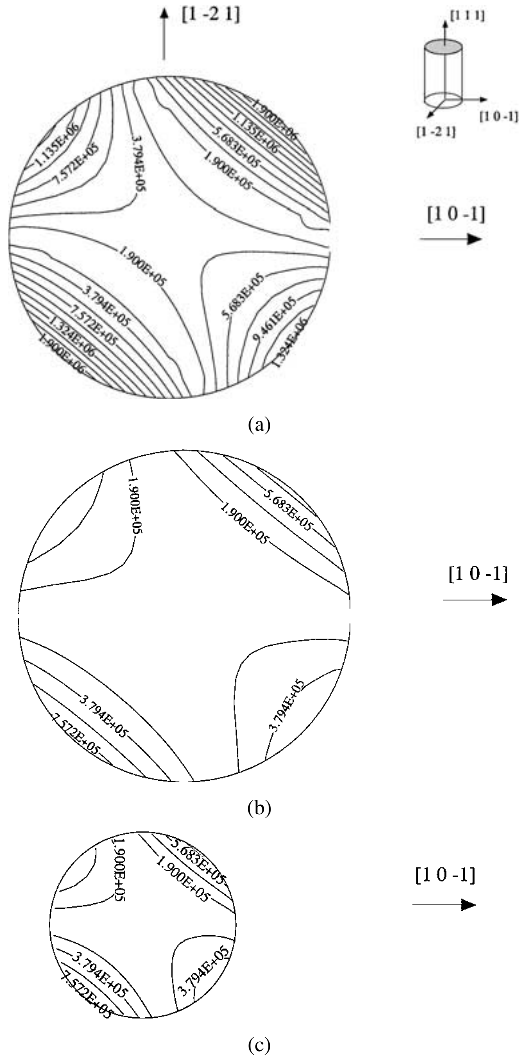


Figure 7 The RSS on (111) plane near the top of the boule for $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$ twinning system for GaAs crystal grown by VGF for cases (a)–(c). The numbers on the contours are in Pa.

show that there are only two different distribution patterns. In Fig. 6b, first one shows the elliptical contour lines through the wafer with high RSS at the center of wafer, after decreasing at the midway, RSS reaches largest value along the short axis of ellipse near the edge of the wafer. Fig. 6a and c show another pattern of two-fold symmetric contour lines, with lower RSS at the center and along the symmetry lines. For each twinning plane, there is always one twinning direction having elliptical contour line stress pattern and two twinning directions having two-fold symmetric contour line pattern. These patterns are observed in crystals grown along both the [001] and the [111] growth directions. For the GaAs crystal grown along the [001] pulling direction, the RSS attains its maximum value of 1.8×10^6 Pa, at the edges of the wafer. The twinning systems having maximum value of stress are the twinning systems having two-fold symmetric with no elliptical stress distribution pattern as shown in Figs. 6a and 6c.

The RSS contour lines for each twinning system near the top of the crystal for GaAs grown for cases (a)–(c) are studied for [111] and [001] crystal growth direction. Results show that RSS values vary with twinning systems. A typical high RSS contour line pattern is shown in Fig. 7 for $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$ twinning system on (111) plane near the top of the boule for GaAs crystal grown for cases (a)–(c), along [111] growth direction. Fig. 7 illustrates that largest RSS, which is about 1.9×10^6 Pa, in the GaAs wafer grown along [111] direction appears normal to the direction lying along the directions at 45° to the $[10\bar{1}]$ and $[1\bar{2}1]$ directions for the area near edge of the wafer. Fig. 7a and b demonstrate that even though the RSS contour patterns are similar, the maximum value of RSS in grown crystal will be reduced more than half (from 1.9×10^6 to 7.5×10^5 Pa) by reducing imposed temperature gradients from −5 K/cm (case a) to −2 K/cm (case b). Fig. 7a and c also show that the maximum value of RSS in 5 cm radius grown crystal is reduced more than half by reducing the radius of crystal from 5 cm (case a) to 2.5 cm (case c). In order to understand the effect of growth direction in different growth parameters, contour lines of RSS on (001) plane near the top of the boule for $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$ twinning system along [001] pulling directions are illustrated in Fig. 8. Results shows that similar effects are obtained by

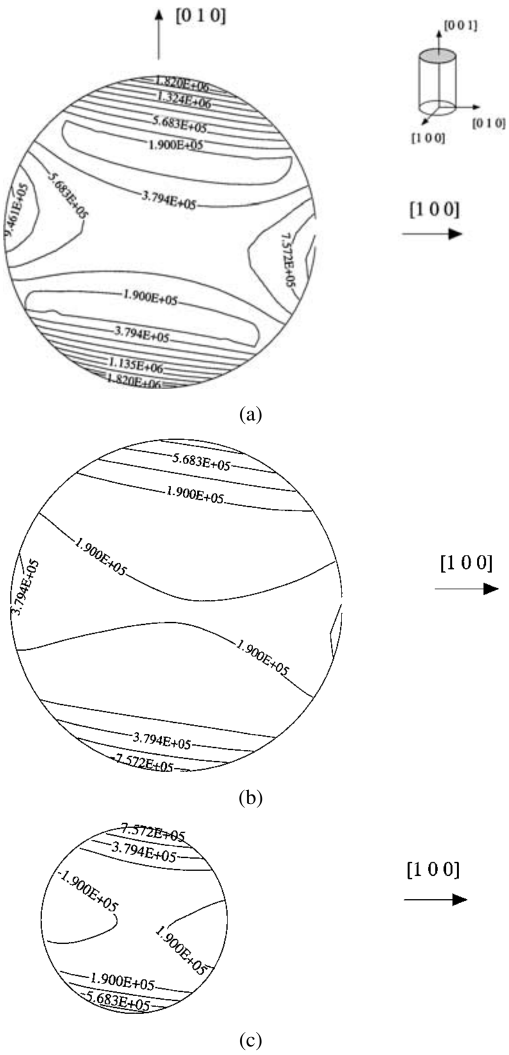


Figure 8 The RSS on (001) plane near the top of the boule for $(\bar{1}1\bar{1})[\bar{2}\bar{1}1]$ twinning system for GaAs crystal grown by VGF for cases (a)–(c). The numbers on the contours are in Pa.

lowering imposed temperature gradient and decreasing crystal radius for crystal grown along [001] direction (see Fig. 8a–c). Figs 7 and 8 illustrate that RSS are always a little larger for crystals grown along the [111] direction for crystals grown at different growth parameters. These results are in reasonable accord with the experimental finding. Experimental evidence [2, 18] has shown that the nucleation of the twins are most likely to occur at larger diameter and higher value of v and start at the edges of the crystal. Another evidence by Chung *et al*. [19] also shown that the occurrence of twins in magnetic liquid encapsulated Czochralski grown InP crystals (According to Hurle [5], InP and GaAs have similar twin formation mechanism) is nucleated at {111} edge facets which were anchored to the TPB. These evidences are in agreement with the prediction of Hurle's twin formation model [5].

4. Conclusion

A quantitative quasi-steady state twinning stress model is developed for predicting the possible deformation twinning in GaAs crystals grown by the VGF. The model shows that a characteristic two-fold symmetric high RSS pattern in some twinning systems has higher possibility of deformation twin formation on (001) and (111) wafers. The calculated RSS in twinning systems in the grown crystal shows that in VGF grown GaAs crystals lowering the imposed temperature gradients on the cylindrical surface during solidification results in a lower RSS. The results also indicate that a decrease in radius of crystal leads to lower RSS at the edge of the wafer. Thus, RSS shows a strong dependence on the imposed temperature gradients and crystal radius. However the RSS shows a weak dependence on the growth direction. If the CRSS for GaAs is greater than the RSS, no thermal stress generated twins will occur. Otherwise, twins could be generated in any twinning system. Numerical models of RSS such as the one presented here, may allow crystal grower to grow GaAs crystals with few deformation twins through the control of furnace temperature profile and pulling direction during crystal growth.

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