Dislocation Reduction in Semiconductor Crystal Growth

X. A. Zhu, Ph.D.
Postdoctoral Fellow, Department of Mechanical Engineering
Florida Atlantic University
Boca Raton, FL 33431, USA.

C. T. Tsai, Ph.D.
Professor, Department of Mechanical Engineering
Florida Atlantic University
Boca Raton, FL 33431, USA.

Abstract
The presence of dislocations not only considerably reduces the lifetime and performance, but also has a major impact on electronic and optical properties of these materials. A finite element model, which couples the microscopic dislocation density to the macroscopic plastic deformation, will be employed to predict the dislocation density generated in the crystal under different crystal growth parameters. The predicted results will be used to investigate the correlation between dislocation generation and crystal growth parameters. It is hoped that the reveal of this correlation will help to improve the current crystal growth process, and to guide future design of an intelligent crystal growth system. This intelligent processing system will enable crystal growers to reduce dislocation density in a semiconductor crystal through the control of growth parameters.

Keywords
Dislocation generation, Semiconductor crystal, Crystal growth, and Thermal stress.

1. Introduction
Microelectronic devices/circuits are key components in computer, telecommunication, wireless communication, aerospace, and biomedical applications. Most microelectronic and photonic devices/circuits are developed by using the specific characteristics of semiconductor materials, such as GaAs, InP, Si, Ge, etc. It is well known that the presence of dislocations in these semiconductors produces dangling bonds [1], which impart electrical activity to the dislocations and affect the carrier concentration and mobility in semiconductors Therefore, dislocations in semiconductor crystals deteriorating performance and stability of microelectronic devices/circuits have to be reduced [2,3].

A transient finite element model has been developed to simulate the crystal grow process during various VGF growth processes developed by using the worldwide known Haasen model [4]. The dislocation generation of GaAs and InP single crystals grown by the VGF process is studied by using this transient
finite element model, the effects of doping impurity atoms on dislocation generation for these crystals are also investigated.

2. Finite Element Modeling of Dislocation Generation

The motion of dislocations controls plastic deformation of crystals. A quantitative model of plastic strain rate, $\dot{\varepsilon}_{ij}^{vp}$, in the diamond cubic structure (D.S.) crystals developed by Haasen and Alexander is given as follows [5]:

$$\dot{\varepsilon}_{ij}^{vp} = N V_0 b \left( \sqrt{J_2} - D \sqrt{\bar{N}} - \tau_d \right)^p \exp(-Q / kT) \frac{S_{ij}}{2\sqrt{J_2}},$$

(1)

where $D$ is a strain hardening factor, $b$ is the magnitude of the Burgers vector of mobile dislocations, $\bar{N}$ is the density of moving dislocations, $J_2$ the second stress invariant, $S_{ij}$ is the deviatoric stress tensor, $Q$ is the Peierls potential, $k$ is the Boltzman’s constant, $V_0$ is a preexponential factor, $T$ is the absolute temperature, $p$ is a material constant, $\tau_d$ is the drag-stress caused by the doping impurity atoms [6,7,8], and Mawley bracket notation $\langle x \rangle$ is defined as $\langle x \rangle = x$ if $x \geq 0$ and $\langle x \rangle = 0$ if $x < 0$. The generation rate of the mobile dislocation is given by [9]

$$\dot{N} = N K V_0 \left( \sqrt{J_2} - D \sqrt{\bar{N}} - \tau_d \right)^P \left( \sqrt{J_2} - D \sqrt{\bar{N}} \right) \lambda \exp(-Q / kT),$$

(2)

where $K$ and $\lambda$ are the material constants. It is common in the III-V compound semiconductors that 60° dislocation has a higher mobility than screw dislocation [10]. There is neither plastic deformation nor dislocation generation if $\left( \sqrt{J_2} - D \sqrt{\bar{N}} - \tau_d \right) \leq 0$. Eqs. (1) - (2) can then be employed into the transient finite element model discussed next to calculate dislocation generation in the crystal grown from the melt.

For GaAs crystals doped with $2 \times 10^{19}$ of P atoms per cm$^3$, the drag-stress has been found as $\tau_d = 10^{4.150 \pm 1.569 \pm 7.47} \text{ Pa}$ [7]. For InP crystals, three different doping levels are used to investigate the influence of doping impurity on dislocation generation. For InP crystals doped with $1.5 \times 10^{17}$ of Ge atoms per cm$^3$ (low Ge doped), the drag-stress has been found to be $\tau_d = 10^{3.224 \pm 2.793 \pm 0.05} \text{ Pa}$. For InP crystals doped with $1.3 \times 10^{18}$ of S atoms per cm$^3$, the drag-stress has been found to be $\tau_d = 10^{2.925 \pm 3.225 \pm 0.00} \text{ Pa}$. For InP crystals doped with $1.3 \times 10^{19}$ of Ge atoms per cm$^3$ (high Ge doped), the drag-stress has been found as $\tau_d = 10^{6.796} \text{ Pa}$ [6,8].

The temperature distributions of GaAs and InP crystals grown by the VGF process are calculated [11] and shown in Figure 1 for growth parameters of $T_d$ (temperature gradient) = -5 K/cm, $R$ (crystal radius) = 3.0 cm, and $v$ (crystal growth rate) = $2.32 \times 10^4$ cm/s. The calculated temperature distributions are then employed to calculate the dislocation densities generated in the doped and undoped GaAs and InP crystals grown by the VGF process.

Since the crystal growth process is a time-dependent process, a transient finite element model has to be developed to calculate dislocation densities generated in the crystals. A transient finite element model has been developed as [11]

$$[K]_n \{\Delta d\}_n = \{\Delta F\}_n,$$

(3)

where

$$[K]_n = \int [B]^T [\hat{D}]_n [B] dV,$$

(4)

and

$$\{\Delta F\}_n = \int [B]^T [\hat{D}]_n \left( \{\dot{\varepsilon}^{vp}\}_n \Delta t_n + \{\Delta \varepsilon^{th}\}_n \right) dV.$$

(5)
In Eqs. (3-4), \( \Delta d \) represents the change in displacement components, \( \Delta \varepsilon^{th} \) and \( \Delta F \) are the changes of the thermal strain and equivalent load during the time interval \( \Delta t = t_{n+1} - t_n \). \([B]\) is the strain-displacement matrix, the viscoplastic material matrix is given by

\[
[D] = [D]^{-1} + \theta \left[ \frac{\partial E^{vp}}{\partial \varepsilon} \right]_{n} \Delta t_{n}^{-1}.
\]  

\([D]\) is an elastic material matrix. In Eq. (6), \( \theta \) is between 0 and 1, where \( \theta = 0 \) represents a fully explicit (or forward difference) scheme, \( \theta = 1 \) represents a fully implicit (or backward difference) scheme, and \( \theta = 1/2 \) represents an implicit trapezoidal scheme. Solving \( \{\Delta d\}_n \) from Eq. (3), the nodal displacement components at time \( t_{n+1} \) are obtained as

\[
\{d\}_{n+1} = \{d\}_n + \{\Delta d\}_n,
\]

and the residual stresses components at time \( t_{n+1} \) are obtained as

\[
\{\sigma\}_{n+1} = \{\sigma\}_n + \{\Delta \sigma\}_n.
\]

The accumulated dislocation densities in the GaAs crystal at time \( t_{n+1} \) are obtained as

\[
(N)_{n+1} = (N)_n + (\dot{N})_n \Delta t_n,
\]

where the rate of dislocation generation is obtained from Eq. (2) at time \( t_n \). The solution procedure is repeated for each time interval until the crystal growth process completes.

3. Results and discussions

Substituting the temperature distributions obtained from Section 2 into the transient finite element code [10] developed based on Eqs. (1-9), dislocation densities in the undoped and doped GaAs and InP crystals grown from VGF processes are calculated.
3.1 GaAs crystal grown at \( T_d = -5 \) K/cm, \( R = 3.0 \) cm, and \( v = 2.32 \times 10^{-4} \) cm/s.

Based on the temperature field obtained from Figure 1(a), dislocation density in the undoped GaAs crystal at each discrete time step of VGF process is calculated. Figure 2(a) shows the dislocation density distribution of GaAs crystal when it grows to 4.8 cm long after 41376 seconds of growth, where the maximum dislocation density is \( 3.22 \times 10^6 \) cm\(^{-2} \). It clearly shows that the maximum dislocation density is located at the upper corner near the outer edge of the final bulk crystal.

Dislocation densities in the GaAs crystal doped with \( 2 \times 10^{19} \) of P atoms per cm\(^3 \) after 41376 seconds of growth are calculated and shown in Figure 2(b), where the maximum dislocation density of about \( 2.51 \times 10^5 \) cm\(^{-2} \) is located near the upper corner of the bulk crystal. It also shows that dislocation densities in the majority of the crystal are low. Figures 2(a) and 2(b) clearly show that doping impurity into GaAs crystals can produce more useful low-dislocation-density crystals than those without doping impurity.

![Figure 2](image)

**Figure 2:** Dislocation density distribution (cm\(^{-2} \)) in (a) undoped (b) P doped GaAs crystals after 41376 seconds of growth.

3.2 InP crystal grown at \( T_d = -5 \) K/cm, \( R = 3.0 \) cm, and \( v = 2.32 \times 10^{-4} \) cm/s.

Based on the temperature distribution obtained from Figure 1(b), dislocation density in undoped InP crystals at each discrete time step of VGF processes is calculated. Figure 3(a) shows the dislocation density distribution in InP crystals when it grows to 4.8 cm long after 41376 seconds of growth, where the maximum dislocation density is about \( 5.81 \times 10^4 \) cm\(^{-2} \). It clearly shows that the maximum dislocation densities are located at the upper corner near the outer edge of the final bulk crystal and low dislocation densities are only found in a small region near the bottom of the crystal.

Dislocation densities in the InP crystal doped with \( 1.3 \times 10^{18} \) of S atoms per cm\(^3 \) after 41376 seconds of growth are calculated and shown in Figure 3(b), where the maximum dislocation density of \( 5.16 \times 10^4 \) cm\(^{-2} \). It also shows that dislocation densities in the majority of the crystal are low. Figures 3(a) and 3(b) clearly show that doping S atoms into InP crystals can produce more useful low-dislocation-density crystals than those without doping impurity.
Dislocation density distribution for the InP crystal doped with $1.5 \times 10^{17}$ of Ge atoms per cm$^3$ after 41376 seconds of growth are shown in Figure 3(c), where the maximum dislocation density of $4.78 \times 10^4$ cm$^{-2}$ occurred at the upper corner of the crystal. It also shows that the dislocation densities in the majority of the crystal are low.

Figure 3: Dislocation density distribution (cm$^{-2}$) in (a) undoped (b) S doped (c) low Ge doped (d) high Ge doped InP crystals after 41376 seconds of growth.
Figure 3(d) shows the dislocation density distribution for an InP crystal doped with $1.3 \times 10^{19}$ atoms per cm$^3$. There is no new dislocation generated during the crystal growth process. The maximum dislocation density in the crystal remains 1 cm$^{-2}$ and a dislocation free InP crystal is grown.

Figure 3(a)-3(d) clearly indicate that doping impurity into InP crystals can produce more useful low-dislocation-density crystals than those without doping impurity.

4. Conclusions

The numerical results obtained from the transient finite element model indicate that doping impurity into GaAs and InP crystals can effectively reduce the numbers of dislocation generated in GaAs and InP crystals and increases the yield of those semiconductor crystals grown by the VGF processes. It can be found obviously that doping impurities produce low-dislocation-density GaAs and InP crystals except the outer edge, which matched well with the experimental observation. The results also show that for InP crystal the number of dislocations generated in the crystals decreases as Ge atoms doped into the crystal increases. When the impurity doped into the InP crystals increases to a certain level, a 100% dislocation free crystal can be grown. However, doping too much impurity into GaAs and InP crystals will reduce the performance of these crystals.

Therefore, this model can be effectively used by crystal growers to investigate the effects of doping impurity on dislocation generation in GaAs and InP crystal grown from the VGF processes or other bulk crystal growth processes. The selection of an acceptable level of doping impurity that produce the lowest dislocation density in GaAs and InP crystals can be obtained through a thorough numerical investigation using this developed transient finite element model.

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References