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Numerical Analysis for Transient Point Defect Behavior in Czochralski Silicon Crystal Growth

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Abstractr–To study the transient point defect distribution in Czochralski-grown silicon single crystals, a continuum model of point defect dynamics to predict the concentration of interstitial and vacancy is established by estimating expressions for the thermo-physical properties of point defects and the point defect distribution in silicon crystals. It is well known that the concentration of intrinsic point defects in growing silicon crystals is a function of the crystal pull rate (V) and the temperature gradient (G) at the solidification interface inside the crystal, and steady state predictions from point defect dynamics are well agreed with experiment. In this study, finite element simulations have been performed for the growth halt experiment with 150 mm silicon single crystals to study the transient behavior of intrinsic point defects. It has been demonstrated that predicted point defect distributions are in good agreement with experimental results.

Key words: Point Defect Dynamics, Numerical Analysis, Finite Element Method, Czochralski, Silicon

INTRODUCTION

The development of silicon wafers whose properties can meet the design rule of advanced devices is a key engineering activity for achieving high device yield and reliability. It is very important to understand and control the intrinsic point defect distributions for the production of high quality crystals. The concentration of intrinsic point defects in Czochralski growth of silicon single crystals has been documented to be a function of the crystal pull rate (V) and the temperature field in the crystal during the crystal growth process [Voronkov, 1982; Hasebe et al., 1989; Ammon et al., 1995; Voronkov and Falster, 1998; Wang et al., 2001]. Therefore, the crystal defects related to intrinsic point defects can be controlled during the crystal growth process by the adjustment of process conditions and the modification of hot zone structures. One of the goals of the transient point defect dynamics analysis reported here is to develop a way to design hot zone configurations for high quality crystals.

It is generally believed that interstitials dominate the crystals at lower crystal pull rate and vacancies are in excess at higher crystal pull rate. These results are in qualitative agreement with the predictions of the empirical V/G correlation. The axial temperature gradient at the melt/crystal interface, G, is in the crystal side. According to the experimental findings [Dornberger and Ammon, 1996; Wang et al., 2001], it can be assumed that vacancy type defects are formed if $V/G > \xi_{crit}$, and interstitial-type defects will dominate for $V/G < \xi_{crit}$. The specific value for the critical V/G (ξ_{crit}) is used as 1.38×10^{-3} $cm^2/min \cdot K$ [Sinno et al., 1997].

The steady state behavior of point defects in Czochralski-grown silicon crystals has been studied by many researchers [Brown et al., 1994; Dornberger and Ammon, 1996; Sinno et al., 1997, 1998; Wang et al., 2001]. Wang et al. [2001] studied the numerical computations to give a detailed picture of the development of the self-interstitial and vacancy distributions in a silicon single crystal during the cooling of crystals in Czochralski growth. Their simulation results for a several crystal pull rate demonstrate the growth of the region of excess vacancy from a crystal dominated by interstitial with increasing V, and interstitial is in excess everywhere at lower crystal pull rate. The steady state predictions from point defect dynamics are in qualitative agreement with experiments and empirical V/G analysis when correlated with the radius of oxidation-induced stacking faults ring. These works gave the basis for direct comparison between simulation and the observation of micro-defect distributions in Czochralski-grown silicon wafers.

In this paper, the application of transient point defect dynamic analysis for abrupt change of the crystal pull rate with 150 mm silicon single crystals is studied.

MATHEMATICAL MODEL

The mathematical model equations to predict the time dependent point defect concentrations were developed and shown in this section. The modeled temperature distributions in the crystal phase were used as input for the calculation of concentrations and thermophysical properties of intrinsic point defects - vacancy and (self-) interstitial such as diffusivity and rate constant of recombination reactions [Wang et al., 2001].

1. Modeled Temperature Distributions

In this work, numerical simulations were carried out by decoupling heat transport and point defect transfer, because the intrinsic point defect concentrations are low enough to do not couple back to heat transport properties. The temperature distributions in the crystal phase for several crystal height used in the transient point defect dynamic analysis are shown in Fig. 1. The temperature distribution in the crystal phase is given as

$$T(r,z) = \exp(-\mu_1 (r/R)^2 z)\left[T_a + (T_m - T_a)\frac{\exp(\mu_2 (z_{top} - z))}{\exp(\mu_2 - z)}\right] \quad (1)$$

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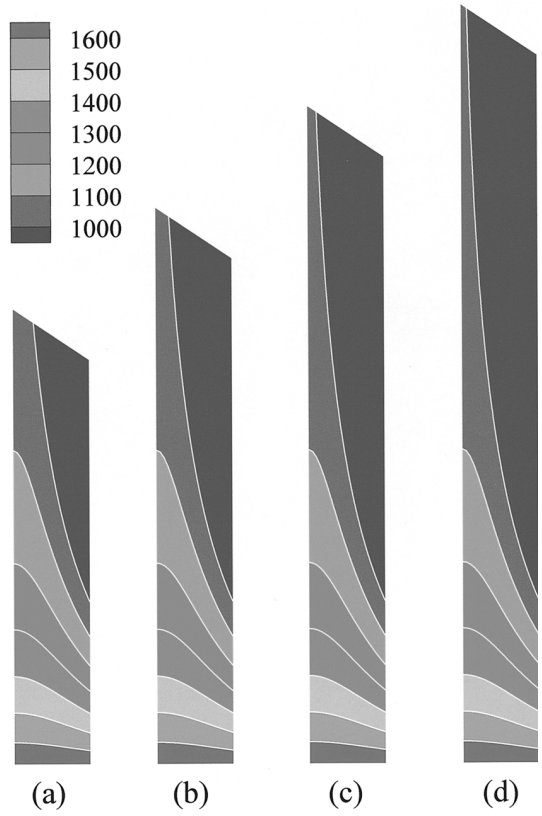

Fig. 1. Temperature distributions used in the transient analysis of point defect dynamics. (a) 40 cm, (b) 50 cm, (c) 60 cm, (d) 70 cm. The isotherms are shown in increments of 100 K between 1,600 and 1,000 K.

$$z_{top}(t) = z_{top}(0) + \int_0^t V(\tau)\,d\tau \quad (2)$$

which contains three parameters (μ_1, μ_2, T_a) and one process condition. The parameters μ_1 and μ_2 control the radial and axial temperature distributions, respectively. T_a is approximately equal to the temperature at the top surface of the silicon single crystal. Calculations reported here are performed with the optimized parameter values μ_1, μ_2 and T_a=1,000 K.

R and T_m are the radius of growing crystal and the melting temperature of silicon material, respectively. V and z_{top} are the crystal pull rate and the silicon single crystal height, respectively.

2. Transient Point Defect Dynamics

Transient conservation equations for the transient change, convection, diffusion and recombination of intrinsic point defects are written in terms of concentration of interstitial and vacancy as

$$\frac{\partial C_I}{\partial t} + V\frac{\partial C_I}{\partial z} = \nabla\cdot(D_I\nabla C_I) + k_{IV}(C_I^{eq}C_V^{eq} - C_IC_V) \quad (3)$$

$$\frac{\partial C_V}{\partial t} + V\frac{\partial C_V}{\partial z} = \nabla\cdot(D_V\nabla C_V) + k_{IV}(C_I^{eq}C_V^{eq} - C_IC_V) \quad (4)$$

C_I and C_V are interstitial and vacancy concentrations computed inside the growing crystal by solving field equations on the basis of modeled temperature. C_I^{eq} and C_V^{eq} are the equilibrium concentrations of interstitials and vacancies, respectively, at the local temperature T of the crystal. D_I and D_V are the diffusion coefficients and k_{IV} is the kinetic rate constant for the rate of recombination of interstitials and vacancies. The cylindrical co-ordinate system (r, z) is centered at the center of the melt/crystal interface. The continuum description of point defect dynamics is completed by supplying expressions for the equilibrium, transport and kinetic parameters. A thermo-physical parameter set of point defects obtained by Wang et al. [2001] is used for the transient point defect dynamic analysis.

The solutions of the transient second order partial differential equations require the initial and boundary conditions. The steady state solutions are used for the initial condition. At the interface, interstitials and vacancies are incorporated at their equilibrium concentration. As the vacancy concentration is 20% higher at the crystallization temperature, the crystals become entirely vacancy rich. We assume that the interstitial and vacancy concentrations are in equilibrium at the melt/crystal interface. The axis of the crystal (r=0) is taken as an axis of symmetry. We also assume that the flux of point defect is zero along the exposed crystal surface.

In this analysis, the enthalpies of formation of the point defects are assumed to be zero. The comparison of steady-state point defect dynamic analysis and experimental results for the position of oxidation-induced stacking faults ring diameter with slow change of crystal pull rate has been discussed in detail by Wang et al. [2001].

NUMERICAL ANALYSIS

The spatial discretization of a complete set of the mathematical model described in the previous section is performed by using the Galerkin finite element method. The intrinsic point defect concentration fields are represented in the expansions of Lagrangian biquadratic basis functions. A computational mesh is formed of quadrilateral elements which span the analysis domains corresponding to the silicon single crystal phase. The governing equations are put into the weak form and boundary conditions are imposed in the normal manner [Wang et al., 1996, 1999].

Implicit Euler method is used for the time-dependent calculations. In the continuum balance equations for the transport and interactions of intrinsic point defects without accounting for the formation of aggregates, the crystal height is changed throughout the Czochralski process. In evaluating the time derivatives, $\partial C_I/\partial t$ and $\partial C_V/\partial t$, we use the procedure developed by Lynch and Gray [1980] to consider the mesh deformation due to the change of crystal height. The detailed numerical methods used in this work are described by Wang et al. [2001], and this approach has proven to be both accurate and robust in a variety of calculations.

RESULTS AND DISCUSSION

1. Experimental Results for Abrupt Change of Crystal Pull Rate

The crystal growth experiments were performed by Kim et al. [2002] to study the transient behavior of intrinsic point defects in 150 mm Czochralski-grown silicon single crystals.

In this work, crystals were grown with a crystal pull rate of $V/G > \xi_{crit}$, until steady state was reached. Then the crystal pull rate was decreased abruptly to $V/G < \xi_{crit}$. The crystal growth was nearly halted at the ingot position of 40 cm for various slow pulling times (30, 60, 120 and 180 min). And the crystal pull rate was increased again to $V/G > \xi_{crit}$. Fig. 2 shows the schematic of crystal pulling

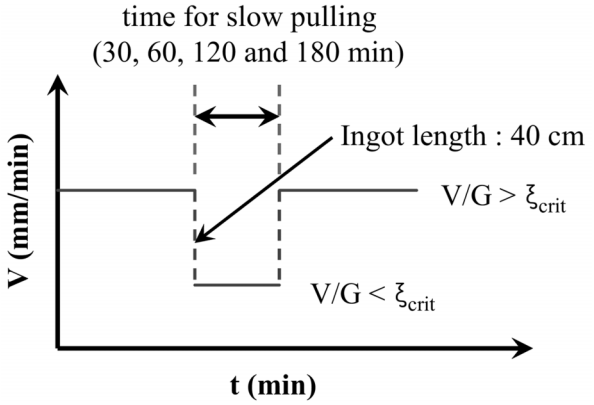

Fig. 2. The schematic diagram of crystal pulling rate near the slow pulling position.

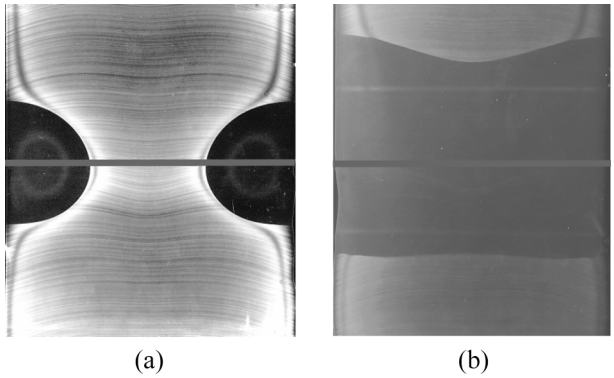

Fig. 3. X-ray topography of an axial section of Czochralski-grown silicon single crystal for slow pulling time of (a) 30 min and (b) 180 min. The diameter of silicon single crystals is 150 mm [Kim et al., 2002].

rate near the slow pulling position. Fig. 3 shows the X-ray topography of a vertical section of 150 mm silicon single crystal for slow pulling times of (a) 30 min and (b) 180 min [Kim et al., 2002]. The X-ray topography (Lang-topography) was measured after the surface oxide layer of the heat treated (950 °C, 30 min) wafer was removed by HF. The solid lines shown in Fig. 3 represent the start position of slow pulling. It is clearly observed that the defect features are not limited to the slowly grown crystal part, but spread into the regions of higher crystal pull rate, which would be completely vacancy-rich under steady state conditions. The interstitial rich region is enlarged with the time of slow pulling.

2. Transient Simulations for the Behavior of Intrinsic Point Defects

Transient point defect concentration fields in the crystal phase were obtained by applying the numerical method to the mathematical model for the Czochralski growth of 150 mm silicon single crystals. A parameter Δ is defined as $\Delta \equiv C_I - C_V$, which is positive for the interstitial dominated part of the crystal. The oxidation-induced stacking faults are assumed to occur at $\Delta=0$, where C_I is equal to C_V.

Predicted transient point defect distributions of crystals at slow pulling time of 30 min are shown in Fig. 4. A steady state distribution of point defects was computed as an initial condition for the

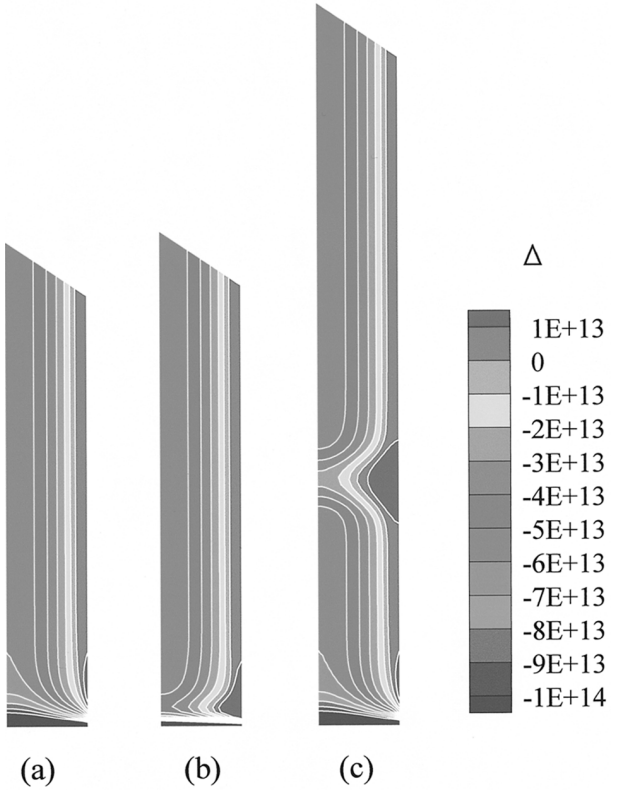

Fig. 4. Simulated point defect distributions Δ of crystals at slow pulling time of 30 min. (a) at the start time of slow crystal pulling, (b) after slow crystal pulling for 30 min and (c) after resuming V/G>ξ_{crit} for 270 min.

transient simulations. During the slow pulling at V/G<ξ_{crit}, the crystal becomes interstitial-rich. The convective transport of point defects is strongly reduced, and diffusive transport becomes important. Diffusion fluxes of point defects are driven by concentration gradient caused by fast recombination. After the slow growth, the strong supply of interstitials overcompensates the vacancy concentration. The crystal becomes interstitial rich near the rim of the crystal close to the melt/crystal interface. When fast pulling is resumed, vacancies are again incorporated in excess into the crystals. The final defect distributions are in agreement with the experimental finding, as the remaining interstitial-rich parts are located near the cylindrical surface.

Simulation results of intrinsic point defect distribution of an axial section of silicon single crystals for slow pulling time of 30 and 180 min are shown together in Fig. 5. Experimental results shown in Fig. 2 [Kim et al., 2002] are well in agreement with these simulations for the transient point defect behavior. For the slow pulling time of 180 min, an interstitial-rich region with a small depression on the top and bottom of the ellipsoid is observed in the experimental and simulation results. The transient point defect dynamics analysis is a useful tool for predicting point defect distributions with changes in operating conditions, such as the crystal pull rate.

CONCLUSIONS

We have performed numerical calculations based on the tran-

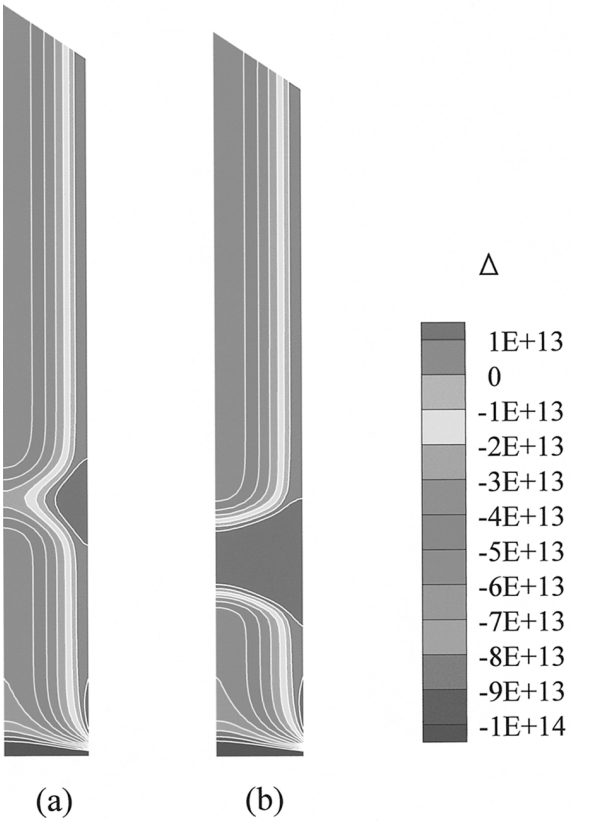

Fig. 5. Simulated point defect distributions Δ of Czochralski-grown silicon single crystal for slow pulling time of (a) 30 min and (b) 180 min.

sient mathematical model which has been developed to describe the intrinsic point defect distributions in Czochralski-grown 150 mm silicon single crystals. The numerical computations give a detailed picture of the development of interstitial and vacancy distribution during the cooling of crystals.

The correct reproduction of the experimental results confirms that the thermo-physical properties, initial and boundary conditions, and other input parameters are very close to the real situations. It is very important to couple the transient point defect dynamic analysis to accurate macroscopic global simulations of heat transfer and melt convection in commercial-scale Czochralski growth configuration. The development of such simulations is underway.

NOMENCLATURE

C_I : concentrations of interstitials [atoms/cm^3]
C_V : concentrations of vacancies [atoms/cm^3]
C_I^{eq} : equilibrium concentrations of interstitials [atoms/cm^3]
C_V^{eq} : equilibrium concentrations of vacancies [atoms/cm^3]
D_I : diffusion coefficient of interstitials [cm^2/sec]
D_V : diffusion coefficient of vacancies [cm^2/sec]
G : axial temperature gradient at the melt/crystal interface [K/cm]
r : radial coordinate [cm]
t : time [sec]
T : temperature [K]
T_a : process condition parameter to account for the ambient temperature [K]
T_m : melting temperature of silicon [K]
V : crystal pull rate [mm/min]
z : axial coordinate [cm]
z_{top} : height of silicon single crystal [cm]

Greek Letters

Δ : characteristic parameter defined as $\Delta \equiv C_I - C_V$ [atoms/cm^3]
μ_1 : control parameter of radial temperature distribution [·]
μ_2 : control parameter of axial temperature distribution [·]
ξ_{crit} : critical value of V/G to predict the position of oxidation-induced stacking fault ring [cm^2/min·K]

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