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Transient analysis of point defect dynamics in czochralski-grown silicon crystals

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Abstract The continuum model of transient point defect dynamics to predict the concentrations of interstitial and vacancy is established by estimating expressions for the thermophysical properties of intrinsic point defects. And the point defect distribution in a Czochralski-grown 200mm silicon single crystal and the location of oxidation-induced stacking fault ring (OiSF-ring) created during the cooling of crystals are calculated by using the numerical analysis. The purpose of this paper is to show that this approach lead to predictions that are consistent with experimental results. Predicted point defect distributions by transient point defect dynamic analysis are in good qualitative agreement with experimental data under widely and abruptly varying crystal pull rates when correlated with the position of the OiSF-ring.

Key words Point defect dynamics, Oxidation-induted stacking faults, Czochralski, Silicon single crystal, Finite element method, Transient analysis, Numerical simulation

1. Introduction

The development of silicon wafer of which properties can meet the design rule of advanced devices is a key engineering activity to achieve a high device yield and reliability. It is very important to understand and control the intrinsic point defects for the production of high quality crystals. It is well known that the concentration of intrinsic point defects in the Czochralski growth of silicon single crystals is a function of the crystal pull rate, V, and the axial temperature gradient, G, at the melt/crystal interface inside the crystal [1-9]. 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 dynamic analysis reported here is to develop the way to design the hot zone configurations for high quality crystals.

The Oxidation-induced Stacking Faults ring (OiSF-ring) is one of the visible boundaries between vacancy and interstitial dominated region and another key issue for understanding the point defects movements. The relationship between the radius of the OiSF-ring and Czochralski process conditions has been studied experimentally and theoretically for steady state conditions with slow change of crystal pull rate by Wang *et al.* [8, 9].

In this paper, the application of transient point defect dynamic analysis for several problems that arises in Czochralski crystal growth is studied. It has been demonstrated that predicted point defect distributions are in good qualitative agreement with experimental results and steady-state point defect dynamic analysis under widely varying process conditions when correlated with the location of the OiSF-ring. In this study, transient simulation has been performed for abruptly varying the crystal pull rates with the 200 mm silicon single crystals to study the macroscopic behavior of OiSF-ring.

2. Mathematical Model

The mathematical model equations to predict the time dependent point defect concentrations were developed and shown in this section. The modelled 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.

2.1. Modelled temperature distributions

We report calculations for 200 mm Czochralski-grown

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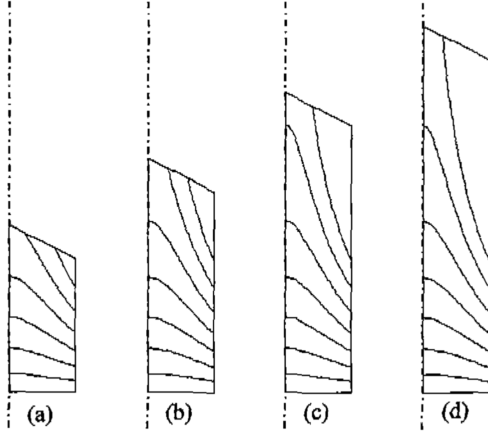

Fig. 1. Temperature field for several crystal height - (a) 20 cm (b) 30 cm (c) 40 cm and (d) 50 cm - used in transient point defect dynamic analysis. The isothermsare shown in increments of 100 K between 1600 and 1000 K.

silicon single crystals. The temperature distributions in the crystal phase for several crystal height as shown in Fig. 1. The temperature distributions in the crystal phase is given as

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

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

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 parameter values $\mu_1 = 0.012$, $\mu_2 = 0.048$ and Ta = 1000 K.

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

2.2. 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

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

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

C_I and C_V are interstitial and vacancy concentrations computed inside the growing crystal by solving field equations on the basis of modelled 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.

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. 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. Additional calculations with equilibrium condition along all exposed crystal surface were performed to study the influence of boundary conditions on the point defect distributions. Other boundary conditions are possible. For example, Brown *et al.* [3] assumed that point defect along the surface of the crystal are in equilibrium at the local temperature.

A thermophysical parameter set of point defects obtained by Wang *et al.* [8, 9] is used for the transient point defect dynamic analysis. In this analysis, the

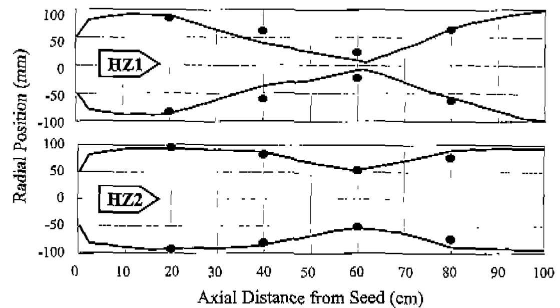

Fig. 2. Comparison of steady-state point defect dynamic analysis and experimental results for several hot zone structures [9]. Solid line and filled circles represent OiSF-ring position obtained by experiment and simulation, respectively.

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 OiSF-ring diameter with slow change of crystal pull rate has been discussed in detail in ref. [9]. The comparison of computational and experimental results of OiSF-ring diameter for several hot zone configurations is shown in Fig. 2, taken from [9]. The simulation results are based on the steady-state point defect dynamic analysis coupled with the global heat transfer analysis.

3. Numerical Analysis

The Galerkin finite element method is used for the discretization of complete set of the mathematical model. The intrinsic point defect concentration fields are represented in expansions of Lagrangian biquadratic basis functions. A mesh is formed of quadrilateral elements which span the computational domains corresponding to the crystal phase. The field equations are put into the weak form and boundary conditions are imposed in the normal manner [10, 11].

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 [12] to consider the mesh deformation due to the change of crystal height. The detailed numerical methods used in this work are de- scribed in ref. [8] and this approach has proven to be both accurate and robust in a variety of calculations.

4. Results and Discussion

Transient point defect concentration fields in the silicon crystal phase were obtained by applying the numerical method to the mathematical model for the Czochralski growth of 200 mm silicon single crystal. The OiSF-ring subdivides the crystal into interstitial rich outer region and vacancy rich inner region. A parameter Δ is defined as $\Delta \equiv C_I - C_V$ which is positive for the interstitial dominated part of the crystal. The OiSF-ring is assumed to occur at $\Delta = 0$, where C_I is equal to C_V

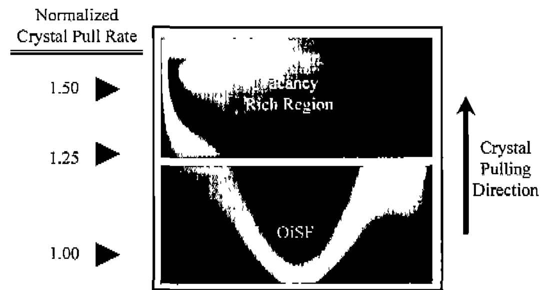

Fig. 3. X-ray topography of an axial section of Czochralski silicon single crystal grown at various crystal pull rates.

Figure 3 shows the X-ray topography of the vertical section of 200 mm silicon single crystals grown at various crystal pull rate with Czochralski method. The X-ray topography (Lang-topography) was measured after removing the surface oxide layer of the heat treated (950°C, 30 min) wafer by HF. The dependence of radius of OiSF-ring on the crystal pull rate is shown in Fig. 3. The radius of OiSF-ring is decreased with the decrease of crystal pull rate. When the crystal pull rate is further slowed down to a specific value, the radius of OiSF-ring contracts toward the center of the crystal and disappears finally.

The qualitative behavior of OiSF-ring with the decrease of crystal pull rate in silicon crystals grown by Czochralski hot zone is studied using the point defect dynamics analysis. Figure 4 shows the experimental data and simulation results for the transient as well as steady state point defect dynamic analysis. In both cases (transient and steady state analysis), the mathematical model and numerical method developed in this work is able to predict well the position of the OiSF-ring as a function of the crystal pull rate.

We attempt to explain the macroscopic behavior of

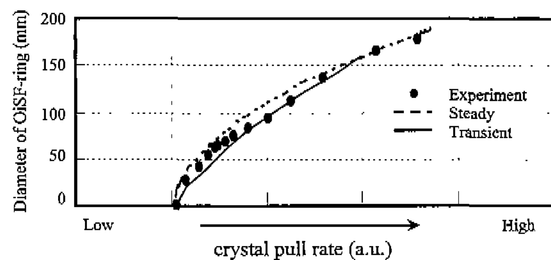

Fig. 4. The effects of crystal pull rate on the diameter of OiSF-ring. Filled circles represent experimental results. The dashed and solid line indicate steady state and transient analysis, respectively.

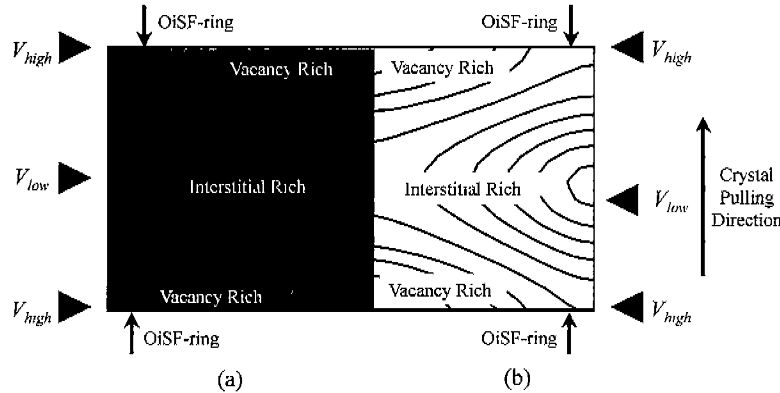

Fig. 5. (a) X-ray topography and (b) simulated point defect distribution (Δ) for the transient analysis. The crystal was grown at lower crystal pull rate for 70 minutes. The diameter of CZ grown silicon single crystal is 200 mm.

OiSF-ring shrinkage with abruptly varying the crystal pull rates using the transient point defects dynamic analysis. The effects of the crystal pull rate on the concentrations of interstitial and vacancy and the location of OiSF-ring are discussed in ref. [8]. At lower crystal pull rate (V_{low}), interstitial is in excess everywhere. And vacancy is in excess at higher crystal pull rate (V_{high}). Under steady state conditions, the type of the prevailing point defect species is exclusively determined by the ratio of crystal pull rate and axial temperature gradient in the crystal phase at the melt/crystal interface. And it has been demonstrated that computed point defect distributions are in good agreement with experimental data for steady or nearly steady state conditions under widely varying process conditions.

In this work, crystal was grown with a crystal pull rate of V_{high}, until steady state has been reached. Then the crystal pull rate was decreased abruptly to V_{low} for 70 minutes and the crystal pull rate was increased again to V_{high}. Figure 5(a) shows the X-ray topography of a vertical section of 200 mm silicon single crystal. 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. Figure 5(b) shows the simulated point defect distribution (Δ) using the transient analysis. The experimental results are well in agreement with the transient point defect dynamic analysis. The transient point defect dynamics analysis is a useful tool to predict the spatial and temporal evolution of OiSF-ring with changes in operating conditions, such as the crystal pull rate.

5. Summary

We have performed numerical calculations based on the transient mathematical model which has been developed to describe the intrinsic point defect distribution in Czochralski-grown 200 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 thermophysical 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.

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