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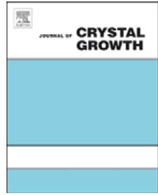

A kinetic model of the formation and growth of interstitial dislocation loops in dislocation free silicon single crystals

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ABSTRACT

A kinetic model of the formation and growth of dislocation loops in course of consequent as-grown crystal's cooling has been proposed It demonstrates that dislocation loops are formed following the processes of high-temperature precipitation of background oxygen and carbon impurities during crystal growth. Elastic deformation caused by growing precipitate is released due to the formation and growth of dislocation loops. Interstitial dislocation loops are formed, when the crystal growth ratio is $V_g/G < \xi_{crit}$. We have compared the kinetic model calculation data with the experimental research findings related to the formation of dislocation loops.

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1. Introduction

Recently, we proposed a model of impurity precipitation in course of dislocation free silicon single crystals cooling after being grown within the temperature range of 1683 to 300 K [1]. It includes the kinetic models of oxygen and carbon precipitates formation, and as well as the kinetic model of their growth and coalescence [2,3]. The model of impurity precipitation in course of crystal growing is based on the experimentally and theoretically established fact that there is no recombination of intrinsic point defects at high temperatures, and there is elastic interaction between impurities and intrinsic point defects [4,5].

Either microvoids or interstitial dislocation loops are formed under specific thermal conditions of crystal growth depending on the growth ratio V_g/G (where V_g is a crystal growth rate, G is an axial temperature gradient) within the cooling temperature range of 1403 to 1223 K [6,7]. The authors of these papers made an assumption of a fast recombination of intrinsic point defects near the crystallization front. From this assumption many researchers have developed different variations of the point defect dynamics model [8–11]. The papers implied only that a homogeneous nature of the formation of microvoids and interstitial dislocation loops, and never allowed for impurity precipitation during the crystal cooling [9].

We calculated the formation of microvoids and interstitial dislocation loops according to rigorous approximation for the point defect dynamics model subject to no recombination of intrinsic point defects at high temperatures [12]. It was proved that the process of microvoid formation has a homogeneous nature. However, the formation of interstitial dislocation loops is determined, mainly, by the deformation mechanism. This conclusion was made on the basis of a three order of magnitude discrepancy between the experimentally observed concentration of interstitial dislocation loops and their estimated value. As a result, there is a need in the development of a kinetic model of the formation and growth of interstitial dislocation loops based on the deformation mechanism. Therefore, the objective of this paper is to develop a kinetic model of the formation and growth of interstitial dislocation loops in course of consequent as-grown crystal's cooling based on the deformation mechanism.

2. Nomenclature of grown-in microdefects

The most of the papers related to the observation of a defect structure of dislocation free silicon single crystals are connected with the study of the point defects interaction during the crystal growing, the clarification grown-in microdefects nature, and as well as identification of interaction between thermal conditions of crystal growth and grown-in microdefects formation. The experimental classification of grown-in microdefects employs the terms such as A-microdefects, B-microdefects, D(C)-microdefects, (I+V)-microdefects and microvoids [5]. The classification

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is based on the use of the methods of preferential etching, X-ray topography and transmission electron microscopy. It was found that A-microdefects constitute interstitial-type dislocation loops, and B-microdefects, D(C)-microdefects, (I+V)-microdefects constitute precipitates of background oxygen and carbon impurities at different stages of their evolution [1,5]. The origin and sizes of precipitates in the silicon lattice are defined by oxygen and carbon concentration in it, and as well as by thermal conditions of single crystal growth [1]. For example, in small-scale FZ-Si single crystals of 30 mm in diameter if the crystal growth rate decreases from 9 to 3 mm/min, then the precipitate sizes increase from the range of 3 to 9 nm ((I+V)-microdefects) to the range of 20 to 50 nm (B-microdefects) [5]. At the same time, the concentration of precipitates changes from the range of 10^{13} to 10^{14} cm^{-3} ((I+V)-microdefects) to the range of 10^{10} to 10^{11} cm^{-3} (B-microdefects) [5]. The detailed TEM-observations of A-microdefects have shown that A-microdefects constitute interstitial dislocation loops or their clusters with sizes ranging from 1 to 40 μm [13,14]. A-microdefect size is inversely proportional to the crystal growth rate. The experimental researches demonstrate the concentration of dislocation loops within two orders of magnitude $\sim 10^6$ to 10^7 cm^{-3} [13,14]. Find more details about the experimental researches of grown-in microdefects in the papers [5,15].

At present, it is difficult to apply the experimental classification, since it is necessary to interpret the terms of every type of the grown-in microdefects for each publication. At the same time, from the physical point of view there are only three types of grown-in microdefects, i.e. impurity precipitates, interstitial dislocation loops and microvoids. Besides, when considering the formation of defects in silicon after processing (post-growth microdefects) the terms such as precipitates, dislocation loops and microvoids are also employed. Therefore, in order to harmonize a defect structure, we propose to switch to the physical classification of grown-in microdefects [15].

3. Model

The kinetics of high-temperature precipitation covers three stages: new phase nucleation, precipitate growth and coalescence stage [1,2]. Precipitates originate from elastic interaction between point defects. They are, initially, present in coherent, elastic and deformable state, when lattice distortions close to the precipitate-matrix boundary are not large, and one atom of the precipitate corresponds to one atom of the matrix [16]. Elastic deformations and any mechanical stress connected with them cause a transfer of excessive (deficient) substance from the precipitate or vice versa. Storage of elastic strain energy during the precipitate growth results in a loss of coherence by matrix. In this case it is impossible to establish one-to-one correspondence between atoms at different sides of the boundary. It results in structural relaxation of precipitates which occurs due to formation and movement of dislocation loops.

To simulate a stress state of the precipitate and the matrix surrounding it, it is sufficient to observe the precipitate which is simple spherical in shape. There can be found analytical solutions in respect of spherical precipitates [17]. Let us take the theoretical and experimental researches of stress relaxation at volume quantum dots as initial model [18–21]. According to these representations, as far as the precipitate grows, its elastic field induces the formation of a circular interstitial dislocation loop of mismatch. This process contributes to the decrease in total strain energy of the system. A growing precipitate displaces the matrix material in the crystal volume. Interstitial atoms form an interstitial dislocation loop near to the precipitate. At the same time, a mismatch dislocation loop is formed on the very precipitate [21]. At the same time, the critical sizes of precipitates, at which formation of dislocations is energy favorable, have the same order as the critical size of dislocation loops [21].

In the volume of silicon the precipitate produces a stress field caused by mismatch between the lattice parameters of precipitate (a_1) and surrounding matrix (a_2) [21]. Then, the intrinsic deformation of the precipitate is defined as described below:

$$\varepsilon = \frac{a_1 - a_2}{a_1} \quad (1)$$

In general, the precipitate intrinsic deformation in the matrix volume can be expressed as follows:

$$\varepsilon^* = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} \delta(\Omega_{pr}) \quad (2)$$

where the diagonal terms constitute a dilatation mismatch between the precipitate and matrix lattices; the other terms are shear components; $\delta(\Omega_{pr})$ is the Kronecker delta. The elastic fields of precipitate (stress σ_{ij} and deformation ε_{ij}) and the field of total displacement are calculated accounting for intrinsic deformation (2) and regions of precipitate localization $\delta(\Omega_{pr})$. The elastic fields of precipitate are calculated according to the known scheme using elastic moduli, elastic Green function or its Fourier transform [20].

Let us consider the easiest model of a spherical precipitate with equiaxial intrinsic deformation, i.e. $\varepsilon^*_{ii} = \varepsilon, \varepsilon^*_{ij} = 0 (i \neq j; i,j, = x,y,z)$. Elastic strain energy of a spheroidal defect rises according to the cube law as the precipitate radius (R_{pr}) increases [21]:

$$E_{pr} = \frac{32 \cdot \pi}{45 \cdot (1-\upsilon)} \cdot J \cdot \varepsilon^2 \cdot R_{pr}^3 \quad (3)$$

where J is the shear modulus; υ is the Poisson's ratio. Starting from a certain critical value of the R_{crit} radius, the elastic strain energy mechanism begins to work. This mechanism results in the formation of a prismatic interstitial dislocation loop [21]. The energy criterion for such mechanism is the $E^{initial} \geq E^{final}$ condition, where $E_{initial}$, E_{final} constitute elastic energy of the system with precipitate before and after relaxation [21].

In respect of a spherical precipitate with equiaxial intrinsic deformation, the calculation of elastic fields of the precipitate is substantially simplified. Let us assume that the intrinsic elastic strain energy of the precipitate before and after the formation of a dislocation loop of mismatch remains constant $E_{pr}^{initial} = E_{pr}^{final}$. Then, a nucleation criterion for mismatch loop can be presented as $0 \geq E_D + E_{prD}$ condition, where E_D is energy of a dislocation loop of mismatch; E_{prD} is energy of precipitate-dislocation loop interaction [21].

For the purpose of assessment let us assume that a dislocation loop of mismatch has equatorial location on the spheroidal precipitate $R_D = R_{pr}$, and intrinsic energy of a prismatic loop is equal [21]

$$E_{loop} = \frac{J \cdot b^2 \cdot R_D}{2 \cdot (1-\upsilon)} \cdot \left(\ln \frac{2 \cdot R_D}{f} - 2 \right) \quad (4)$$

where f is the radius of the core loop; b is the magnitude of the Burgers vector. A critical value of the precipitate radius corresponds to a value at which the loop is formed on the precipitate [21]

$$R_{crit} = \frac{3b}{8\pi(1+\nu)\varepsilon} \left(\ln \frac{1.08 \alpha R_{crit}}{b} \right) \quad (5)$$

where α is a constant contribution of the dislocation core. Formula (5) is approximate and can be used only to determine the value of R_{crit} critical radius.

This paper [22] theoretically considers the increase kinetics for dislocation loops at the stages of loop growth and coalescence.

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