Simulation of Dislocation Accumulation in ULSI Cells of Reduced Gate Length

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Abstract. We numerically evaluate the accumulation of dislocations in periodic structure of the shallow trench isolation (STI) type ULSI cells which has generally been adopted as the latest semiconductor device structure. STI type ULSI cells with gate length less than 62 nm and various trench depths are employed and subjected to a temperature drop from the initial value of 1000 ℃. Dislocation accumulation is evaluated by a technique of crystal plasticity analysis. Relations between the geometry of the STI type ULSI cells and dislocation accumulation are discussed.

Introduction

In recent years, high-density memories and high-speed CPUs are usually realized by a reduction of the size of semiconductor cells in LSIs. Representative length scale of ULSI cells is going to be at a nano-meter order and the atomic level defects, such as uneven oxidation film or lattice defect generation etc., are becoming more and more important. Among them, dislocations which often appear near hetero-interfaces and accumulate in the electron channel have an enormous effect on the electronic state of the device, increase the signal delay and obstruct devices from normal operation. Therefore, the evaluation and control of dislocations are crucial not only for the design of cell structure but also for the design of process through which ULSI chips are produced. The periodic structure of the shallow trench isolation (STI) type ULSI cells are generally adopted as the latest semiconductor device structure. A lot of investigations have been made on this type of structure and dislocation accumulation is known to be caused by thermo-plastic deformation in silicon during the processes of device fabrication, but detailed aspects on dislocations and their density distribution in the cells are not fully understood. So far, we have analyzed thermal stress, plastic slip deformation, accumulation of dislocations and their structures during the cooling process of STI type ULSI cells by using a technique of crystal plasticity analysis [1]. In these analysis, we employed a numerical model with the gate length of 62 nm. In this study, we introduce some models with different trench geometory and reduced gate length. Thermal stress, plastic slip deformation and accumulation of dislocations in these models during the temperature drops from 1000 ℃ to room temperature are analysed.

Model for numerical analysis

Fig. 1(a) schematically shows the periodic structure of the STI type ULSI cells. One unit of the periodic structure is cut out and we employ it for the numerical analyses. Fig. 1 (b) shows the

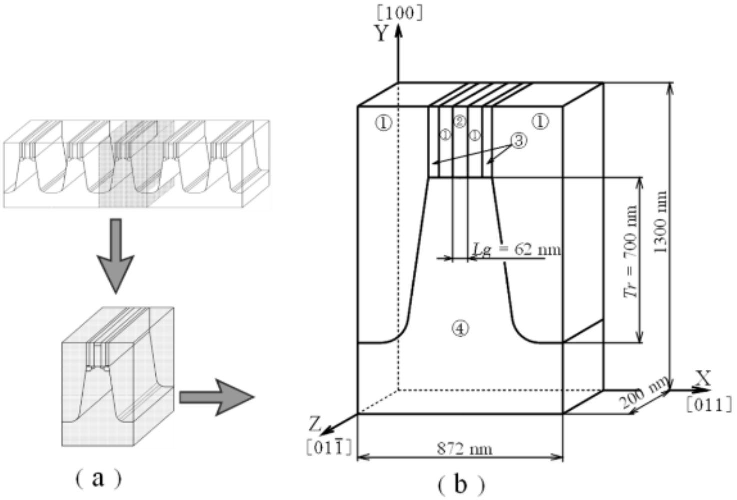

Fig. 1 (a) Schematic illustration of the periodic structure of STI type ULSI cells.
(b) Base-Model employed for crystal plasticity analysis.

base-model used in the analyses. Dimensions of the model are typical for an STI structure with a gate length L_g = 62 nm and trench depth T_r = 700 nm. The structure consists of volumes ① to ④ as shown as shown in Fig. 1 (b). Volumes ① , ② and ③ correspond to buried oxide, gate electrode, and source/drain electrodes, respectively, and for simplicity their materials are assumed to be SiO_2. Volume ④ represents the Si substrate. Crystal orientation of the model is also shown in Fig. 1 (b). The normal of the Si substrate (Y axis) corresponds to the [100] direction, and the trench direction of the STI structure is parallel to the $[01\bar{1}]$ direction.

Models with 34 combinations of different trench depth and gate length are developed by modifying the geometry of the base model. Fig. 2 shows some of the developed models. The first and second numbers shown with a model gives the gate length and trench depth in the unit of nm, respectively. The models are divided into finite elements of the eight node composite type. The numbers of elements and nodes in each model are 10062 and 13920, respectively.

The movement of dislocations and onset of plastic slip deformation are primarily controlled by lattice friction stress. The lattice friction stress is known to depend on deformation temperature, but as far as the authors know, experimental data are not obtained yet. While, the hardeness of Si at different temperatures from 24 to 800 ℃ were obtained by Yonenega et al. [2]. In this study, we assume that the lattice friction at 800 ℃ and above is 30 MPa. At lower temperature than 800 ℃,

Table 1 Material data used in the analyses

Material	Elastic compliances [10^{-11} m^2/N] [3]		
Si	S_{11} = 0.7685	S_{12} = -0.2139	S_{44} = 1.2563
SiO_2	S_{11} = 1.3698	S_{12} = -0.2327	S_{44} = 3.2051

Material	Thermal expansion coefficient [1/K] [3]
Si	2.50×10^{-6}
SiO_2	0.35×10^{-6}

Temperature [℃]	24	100	200	400	600	800	1000
Material	Lattice friction stress [MPa] [1]						
Si	306	294	279	168	78	30	30
SiO_2	10.0×10^3						

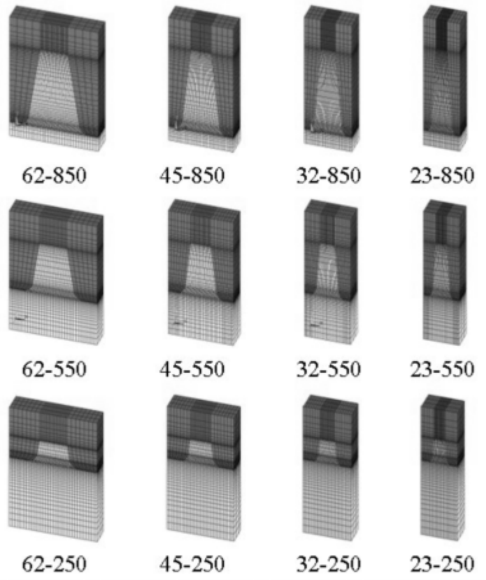

Fig. 2 Numerical models employed for the analysis models.

temperature dependense of the lattice friction is assumed to be the same to that of the hardeness data.

Plastic deformation of SiO_2 is not observed at temperature range lower than 1000 ℃ and we assume a sufficiently high value of lattice friction for this material. Table 1 summarizes material data used in this study.

Crystal plasticity analysis

Plastic slip occurs on the {111} slip plane in the <110> slip direction and there are 12 combinations of slip plane and slip direction, which define the 12 slip systems. Dislocations which accumulate after plastic slip are categorized into two types: statistically stored dislocations (SS dislocations) and geometrically necessary ones (GN dislocations). SS dislocations represent the ones that are trapped by randomly distributed implicit obstacles in the microstructure, and we do not need to consider them in this paper since the Si area is supposed to be a perfect crystal before deformation. In this paper, we study the accumulation of geometrically necessary dislocations. In three-dimensional spaces, the density norms of geometrically necessary dislocations are given by following eqs. [4,5]:

$$\rho_{G,edge}^{(n)} \cdot \tilde{b} = -\frac{\partial \gamma^{(n)}}{\partial \xi^{(n)}} \quad , \qquad \rho_{G,screw}^{(n)} \cdot \tilde{b} = \frac{\partial \gamma^{(n)}}{\partial \zeta^{(n)}} \tag{1}$$

$$\left\| \rho_G^{(n)} \right\| = \sqrt{\left(\rho_{G,edge}^{(n)}\right)^2 + \left(\rho_{G,screw}^{(n)}\right)^2} \tag{2}$$

where $\rho_{G,edge}^{(n)}$ and $\rho_{G,screw}^{(n)}$ denote edge and screw components of the GN dislocations, and superscript (n) denotes the slip system number. The characteristic angle ϕ between the line segment of a GN dislocation and Burgers' vector is given by the following eqs. [4,5]:

$$\sin\phi = \frac{\rho_{G,edge}}{\|\rho_G\|} \quad , \qquad \cos\phi = \frac{\rho_{G,screw}}{\|\rho_G\|} \quad . \tag{3}$$

When ϕ is 0 for example, the segment has a positive screw character, and when $\phi = \pi/2$, the segment has a positive edge character. Plastic slip deformations on 12 slip systems are analysed and density distributions of the geometrically necessary dislocations on these slip systems are evaluated by eqs. (1)-(3).

Results and discussion

When the temperature drops from the initial temperature (1000 ℃), dislocation accumulation occurs on eight slip systems. There are two categories in terms of shape of dislocation accumulation, and four slip systems belong to each category[6]. In the following discussion, we focus on dislocations on the $(11\bar{1})[1\bar{1}0]$ slip system.

Fig. 3 show numerical results for the density distribution of geometrically necessary dislocations when the temperature is 600 ℃. Longer and thicker line segments represent higher density of dislocations. Directions of line segments are calculated by eq. (3). Dislocations shown in Fig. 3 make up half-loop-shaped structures at the bottom corners of the trench and at the shoulder part of the device area. When the trench depth is smaller, dislocation accumulations are enhanced at the bottom corner of the trench and shoulder part of the device area. Therefore, the trench depth is a key parameter for the controll of dislocation accumulation.

Fig. 4 show the average density of dislocations as a function of trench depth and gate length when the temperature is 700℃. We define the average density of dislocations on each slip system by the following equation:

$$\|\rho_G\|_{ave}^{(n)} = \frac{\sum_i \left\| \rho_G^{(n)} \right\| \times v_i}{V} \tag{4}$$

where, v_i is the volume of finite element i, V is the volume of the whole model, and superscript (n) denotes the slip system number. When T_r = 850 or 700 nm, change of the average density of dislocations with the reduction of gate length is not large. However, the average density becomes to increase rapidly with the reduction of the gate length when T_r is smaller than 550 nm. Comparison of data shows that shallower trench results in higher density of dislocations. The effect is prominent especially when the gate length is smaller.

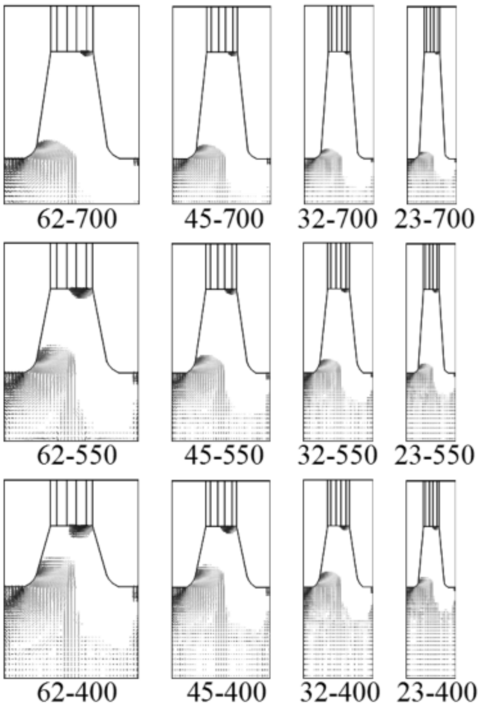

Fig.3 GN dislocations accumulated on the No.07 slip system when the temperature is 600℃.

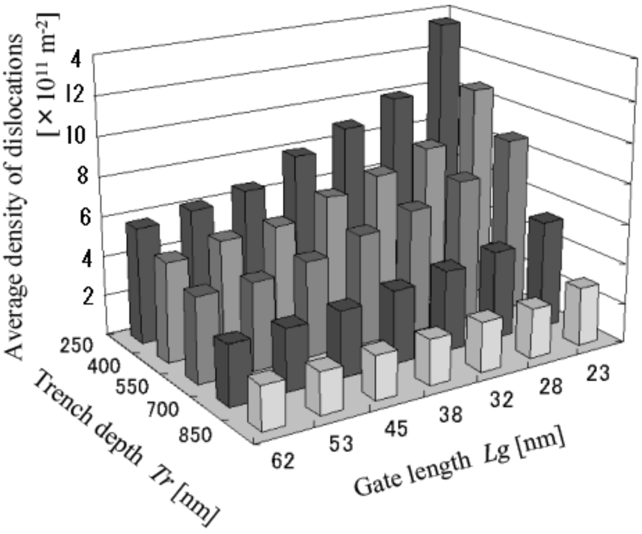

Fig.4 Average density of dislocations depicted as a function of trench depth and gate length when the temperature is 700℃.

Summary

Numerical models of shallow trench isolation (STI) type ULSI cells with various combinations of gate length and trench depth were developed. Thermo-plastic deformation of the models due to temperature drop from 1000 ℃ were analysed using a finite element crystal plasticity technique and accumulation of geometrically necessary dislocations were evaluated. Results showed that reduction of gate length and trench depth both caused an increase of dislocation density.

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