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The use of numerical simulation to predict the unlocking stress of dislocations in Cz-silicon wafers

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Abstract

Under certain conditions, interstitial oxygen atoms in Czochralski-grown silicon (Cz-Si) are known to hinder or completely stop dislocation motion. As a result, oxygen impurities can remarkably improve the mechanical strength of silicon wafers as they are transported and bound to dislocations. The amount of oxygen bound to dislocations—and with it the wafer's resistance to plastic deformation—is oxygen concentration, time, temperature and, importantly, thermal history dependent. It is also reversible. A numerical model has been developed to predict the shear stress necessary to move glide dislocations in Cz-Si wafers during the course (time evolution) of different heat treatments and sequences of heat treatments typical of integrated circuit fabrication. This model accurately accounts for the experimentally observed behaviour of isolated straight dislocations over a wide range of controlled conditions. Modifications to heat treatments can be predicted by using this numerical simulation so that wafer warpage can be minimised during device processing.

Keywords: Silicon; Wafers; Dislocations; Locking; Stress

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1. Introduction

In the semiconductor device industry it is well known that dislocation motion and subsequent plastic deformation of Czochralski-grown silicon (Cz-Si) wafers can occur at high temperatures during device processing [1]. Thermal stresses must be taken into account during the fabrication of integrated circuits since these stresses can generate glide dislocations that produce leakage current in transistors [2] and can seriously compromise the functionality of devices [3].

At high temperatures, gravitational stresses also become important for large diameter wafers (300 mm or more) since they cause plastic deformation especially in areas which are in contact with the wafer holder [4]. Interstitial oxygen atoms can increase remarkably the strength of silicon crystals under appropriate heat treatments [5]. It is experimentally known that Cz-Si shows higher resistance against slip than Float-Zone silicon [6] (FZ-Si) and this difference can be explained in terms of the lack of oxygen in FZ crystals. Typical concentrations

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of oxygen atoms in commercial Cz-Si wafers are of the order of 10^{17}–10^{18} cm^{-3} whereas concentrations in FZ-Si are under the detection limit [usually 10^{15} cm^{-3} with Fourier transform infrared spectrometry (FT-IR)].

During thermal treatments at high temperatures, the formation of oxide precipitates in Cz-Si leads to wafer softening since glide dislocations are generated by stresses arising from the misfit between the oxide precipitates and the silicon matrix [7]. On the other hand, these oxide precipitates (and related dislocations) are important as they act as gettering centres for metallic impurities. The presence of such gettering defects is actually a requirement for very-large-scale integration (VLSI). Therefore, it is extremely important to suppress motion of any pre-existing dislocations either associated with the oxide precipitates or arising from device processing.

The exact mechanism by which glide loops are generated from bulk precipitates is still not completely clear since the different theories developed in the past are still unable to explain all the experimental results. However, from a practical point of view, even if the external stresses are sufficient to start the motion, the dislocations need a certain time to reach the surface or the device active area (depending on their velocity) and it is still possible to control the process [8]. The simplest way to stop the movement of dislocations produced by precipitates or other effects is locking them by segregation of interstitial oxygen atoms which are already present in Cz-Si [9]. The shear stress needed to activate the glide process for a dislocation pinned by oxygen atoms, usually called the ‘‘unlocking’’ stress, depends on the temperature and the number of interstitial oxygen atoms which have diffused to the dislocation core. By understanding and modelling the behaviour of the oxygen atoms at the dislocation core we can predict the unlocking stress necessary to start dislocations moving during a certain heat treatment of the wafer. The strength of the wafer is assumed to be determined by the unlocking stress of the dislocations already present in the bulk. If thermal and gravitational stresses are controlled and kept below the predicted unlocking stress, then no dislocations should glide and plastic deformation of wafers should not occur.

2. The numerical simulation

2.1. Overview

Dislocation cores represent reduced energy sites for interstitial oxygen atoms and thus will tend to be occupied by a higher concentration of oxygen impurities than that present in the bulk. The migration of oxygen to dislocations to produce the increased concentration is controlled by diffusion which is assisted by the interaction of oxygen atoms with the strain field surrounding the dislocation. Consider a dislocation lying along the z axis of an orthogonal coordinate system; the diffusion of oxygen to the dislocation will occur in the xy planes if the oxygen concentration is uniform in the z direction. In this case the system can be described by Fick’s equation for stress-assisted diffusion:

$$\frac{\partial C}{\partial t} = D \nabla \left[\nabla C + \frac{C \nabla (\Delta G)}{kT} \right] \tag{1}$$

where C is the oxygen concentration, D is the oxygen diffusivity, k is Boltzmann’s constant, T is the absolute temperature and ΔG is the Gibbs free energy (binding energy) of the interaction between an oxygen atom and a dislocation. At a given temperature ΔG is given by the thermodynamic relationship:

$$\Delta G = \Delta H - T\Delta S \tag{2}$$

where ΔH is the enthalpy change and ΔS is the entropy change due to the interaction between oxygen atoms and the dislocation.

Eq. (1) becomes one-dimensional with only one independent variable (the radius r) when it is expressed in the usual cylindrical coordinates with the dislocation placed along the cylinder axis. Boundary conditions for Eq. (1) are considered as follows. The first boundary condition can be written as:

$$C(R) = C_0 \tag{3}$$

where R is the minimum distance from the dislocation core at which the oxygen concentration C does not significantly change for the annealing times and temperatures concerned and is equal to the initial oxygen concentration C_0. For the other boundary condition we assume that the dislocation core has a radius r_0 which is taken to be 5 Å [10]; the flux at the boundary $r = r_0$ comprises two terms, one for the absorption and one for the emission of oxygen atoms. In the case of the absorption, incorporation of oxygen to the dislocation is a function of the oxygen concentration adjacent to the core (C_d) and the concentration of available sites (C_a) and oxygen-occupied sites (C_c) at the core. On the other hand, emission of oxygen from dislocations depends on the oxygen concentration in the core C_c and the energy barrier ΔG (the binding energy) to leave the core.

Thus, the net flux J to the dislocation across the boundary at $r = r_0$ can be written as:

$$\mathbf{J}\cdot\mathbf{n}|_{r=r_0} = 2\pi r_0 D\left[C_d\frac{C_a - C_c}{C_a} - C_c\exp\left(\frac{\Delta S}{k}\right)\exp\left(-\frac{\Delta H}{kT}\right)\right] \quad (4)$$

where $\mathbf{n}$ is the unit vector normal to the core [11].

The distribution of oxygen atoms throughout the material and the concentration of oxygen atoms at the dislocation core is deduced from Eqs. (1) and (4) using the finite difference method. The calculation begins by assuming a uniform concentration of oxygen throughout the material, initially equal to C_0, and progresses using small time steps after each of which the entire oxygen distribution is recalculated.

Further details about the equations above and their solution can be found in Ref. [11]. One advantage of using finite difference methods is that the wafer temperature can be changed during the calculation to model the real processes of semiconductor device fabrication.

The simulation outputs the number of oxygen atoms N_c per unit length of dislocation core which is considered to be a cylinder of section πr_0^2.

Experiments have shown that at a certain temperature T, the unlocking stress τ_u is proportional to the number of oxygen atoms at the dislocation core such that:

$$\tau_u(T) = \tau_0(T)N_c \quad (5)$$

where τ_0 is a value equal to the unlocking stress for unit concentration of oxygen atoms. The value of $\tau_0(T)$ was found to vary linearly with the temperature, according to our experimental data in the range 450–650 °C; the empirical expression for $\tau_0(T)$ can be written as:

$$\tau_0(T) = -0.07T + 64.61 \ \ [\mathrm{Pa\,cm}] \quad (6)$$

where T is the absolute temperature. Above 650 °C the unlocking stress τ_0 was found to be approximately independent of temperature. Data about the temperature dependence of τ_0 will be reported in another paper [12].

It has been found that the calculated data for the unlocking stress are in very good agreement with previously published experimental results [13].

2.2. Discussion

It should be noted that the model described above has been developed for isolated, straight dislocations. However, in many practical situations this model may not be appropriate. In the case of dislocations associated with oxide precipitates, the interstitial oxygen concentration is locally depleted and thus the value for C_0 would be lower than that measured for the wafer as a whole. Similarly, if dislocations are present in a surface layer fully depleted of oxygen atoms, then a negligible locking effect can be expected. In some circumstances, where dislocation tangles are developed, the dislocation spacing may be sufficiently small that each dislocation segment can compete in the process of oxygen gettering and this should be considered in a more complicated analysis. Nevertheless, even if the values predicted in the case of straight isolated dislocations are not quantitatively accurate when applied to other particular situations, it is likely that the general trend as to how wafers can be strengthened or weakened according to processing will still be valid.

3. Results

The numerical simulation described above can be used to calculate the dislocation unlocking stress, given by Eq. (5), during a particular heat treatment. The stress necessary to unlock the dislocations varies with duration of thermal treatments and with temperature depending on the amount of oxygen atoms segregated to the dislocation core. The prediction of the evolution of unlocking stress during a specific heat treatment will provide information about the strength of the wafers throughout the processing. In practice, time–temperature profiles are often modified to minimise spatial temperature profiles and thus the thermo-mechanical stresses in wafers being processed. As is shown below, this analysis demonstrates that such modifications affect not only the stresses applied to wafers but also the resistance of wafers to such stresses. The strength of a wafer depends very sensitively on its thermal history; in some cases, different thermal treatments can be proposed to increase the mechanical strength of wafers and hence reduce their susceptibility to warpage. If (time dependent) external stresses are kept below the (time dependent) unlocking stress then plastic deformation of wafers could be prevented. This represents an additional, potentially very useful, independent process control variable.

The numerical model allows the input of several parameters like the initial oxygen concentration, temperature and duration of the annealing steps; by changing these parameters it is possible to simulate the effect of different treatments on the mechanical properties of wafers.

Simple examples of different heat treatments are given below. However, the numerical model could easily be applied to the more complicated treatments used in real device fabrication and would then give an indication of the strength of wafers at any time during their processing. In the following simulations, where not specified, it is assumed that Cz-Si wafers have an initial oxygen concentration equal to 6.3×10^{17} cm^{-3}, although this parameter can be changed and given as input to the model.

The graph in Fig. 1a shows the simulated behaviour of the unlocking stress in a wafer which has been subjected to a particular thermal sequence: this consisted of an increasing temperature ramp (20 °C/min up to 950 °C) followed by a constant temperature step (5 min at 950 °C) and a final cooling step (20 °C/min down to 25 °C). According to calculations shown in Fig. 1a, during the increasing temperature ramp the value of the unlocking stress is initially negligible because the oxygen atoms at low temperatures move very slowly and do not have time to reach the dislocation core in significant numbers. The unlocking stress than increases steeply as the

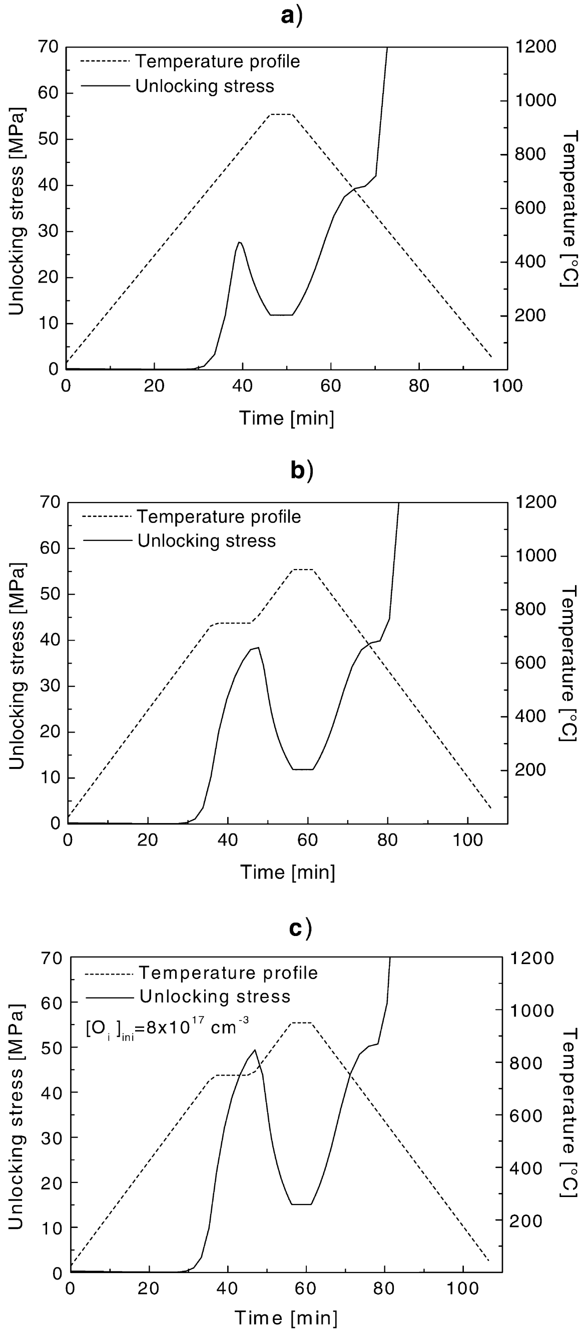


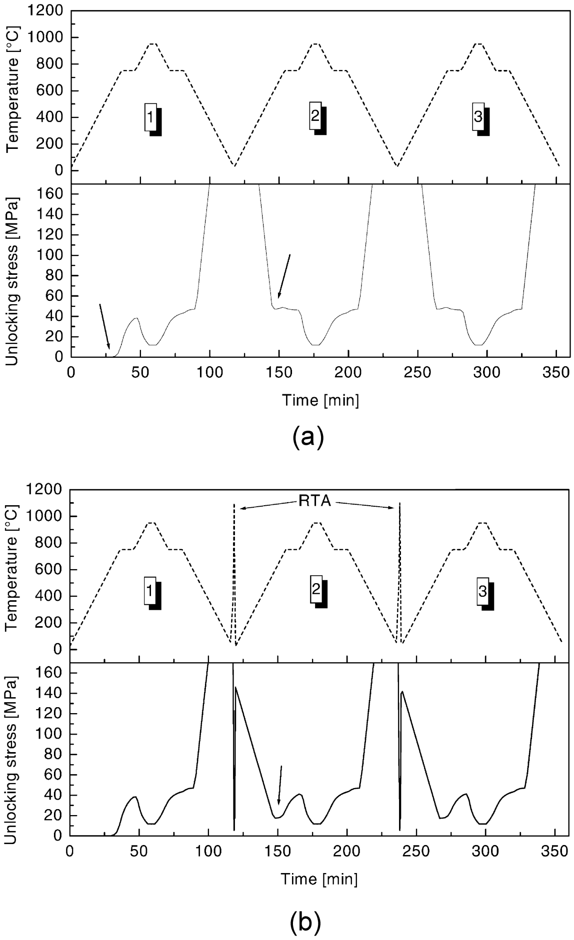
Fig. 1. (a) Unlocking stress behaviour during a specific thermal treatment. (b) Enhancement of the unlocking stress is achieved by introducing an additional annealing step at 750 °C. (c) The dislocation locking can also be improved by simply increasing the initial oxygen concentration in the wafer, for example, to 8.0×10^{17} cm^{-3}.

wafer temperature is raised from 700 to 800 °C and diffusion becomes much more rapid; it subsequently decreases with almost the same slope until the constant temperature step at 950 °C takes place. The decrease is due to the enhancement at higher temperatures of the emission of oxygen atoms from the dislocation core which dominates over the absorption process.

In the final temperature step, during the wafer cooling, the unlocking stress starts increasing again, as more oxygen is absorbed to the core, and rises until room temperature is reached. Therefore, the unlocking stress profile shown in Fig. 1a suggests that at a given stress, for this particular heat treatment, plastic deformation is more likely to occur during the heating of wafers rather than during the cooling when the unlocking stress is larger.

In another sequence shown in Fig. 1b, a pause in the heating ramp has been introduced at 750 °C. In this case the calculation shows that the additional annealing treatment at 750 °C for 10 min allows the unlocking stress to reach a maximum value during the heating which is approximately 11 MPa higher than the previous value obtained. This is an important result if we consider that thermal stresses during device processing are in general not very high and the increase in the unlocking stress of even a few MPa is important because it could lead to a significant reduction of mobile dislocations. Moreover, the unlocking stress can also be substantially increased when a higher oxygen concentration is initially present in the wafers as shown in Fig. 1c.

The simulated behaviour of the unlocking stress during repeated thermal cycles is shown in Fig. 2. Three sequential equal heat treatments are shown in Fig. 2a; the same treatments are shown in Fig. 2b where additional rapid thermal annealing (RTA, up to 1100 °C in 1 min) treatments have been performed. Comparing the two different data plots of the unlocking stress, it was found that the RTA treatment results in a detrimental effect on the wafer strength. Fig. 2a shows that the unlocking stress calculated during the heating ramp in cycle 2 is much higher than that calculated for the same ramp in cycle 1: this is due to the oxygen atoms gathered at the dislocation core during the wafer cooling at the end of cycle 1. Hence, the wafer strength during the heating ramp in cycle 2 will be higher than in cycle 1 (Fig. 2a) for temperatures below 750 °C. This improvement in the strength, obtained during the wafer cooling, is largely lost when RTA is applied just after cycle 1 and before cycle 2 (Fig. 2b). Despite of the short duration of RTA, the significant loss in the magnitude of the unlocking stress is due to the rapid emission of oxygen atoms from the dislocation core at high temperatures. Therefore, according to calculations, during sequential thermal treatments silicon wafers are more susceptible to plastic deformation when subjected to heating ramps which are preceded by an RTA treatment.



(a)

(b)

Fig. 2. Variation of the unlocking stress during repeated thermal cycles when RTA is inserted in between two identical sequences. Arrows indicate the region in the heating ramps where the unlocking stress changes significantly.

4. Conclusions

Interstitial oxygen impurities can improve the strength of Cz silicon wafers by diffusing to the core of stationary dislocations during thermal treatments at high temperatures. The higher the oxygen concentration at the core, the higher the shear stress required to move the dislocations (unlocking stress), and hence the less likely the wafer is to warp. The resistance of a wafer to plastic deformation at any point in time depends on the number of oxygen atoms at the core *at that point in time*. This depends strongly on the oxygen concentration of the wafer and thermal path the wafer has taken up to this point, its thermal history.

A numerical simulation has been developed to estimate the unlocking stress necessary to produce mobile dislocations in Cz silicon wafers. At low temperature, the unlocking stress and hence crystal strengthening is limited by oxygen diffusion and then annealing treatments of long duration are needed to detect a substantial hardening effect. At high temperature, the emission of oxygen from the dislocation core becomes dominant and thus few oxygen atoms are present at the core for dislocation pinning; under these conditions, warpage is more likely occur.

It has been shown that simulated annealing treatments of sufficient duration and at specific temperatures can lead to a remarkable improvement of the mechanical strength of silicon wafers. In the same way the wafers can be weakened by using inappropriate thermal steps. It is thought that the present model may be a useful tool to predict modifications to heat treatments so that wafer warpage may be reduced during device processing.

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