A Prototype Wafer Processing TCAD Tool Composed of BMD Simulation Module, Metal Gettering and Thermal Stress/Slip Functions for Scaled Device Design Phase

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Abstract

We developed a new prototype TCAD tool for wafer processing, particularly to predict BMD(bulk micro defects) distribution, metal gettering characteristics, stress/slip behaviors from the view points of industry such as device reliability and reproducibility. We present herein (i)system concepts and basic models of the tool, (ii)notable output results of BMD radius/profiles in terms of initial interstitial oxygen ([O_i]) concentration and process sequences in conjunction with metal gettering and typical stress/slip behaviors. We also discuss thermal budget customization with emphasis on substrate stiffness and gettering efficiency for reliability and reproducibility improvements in scaled devices.

1 Introduction

With the advent of low thermal budget facilities (RTP), several kinds of Si index substrates, novel high-k dielectrics etc., more aggressive and feasible research on scaled novel devices has been initiated[1]. However, from the view-points of industry such as reliability, reproducibility and cost reduction, technical issues concerning wafers such as process-induced slips, gettering efficiency, wafer thermal stress in the case of larger diameter and BMD have yet to be resolved. In light of this situation, we developed a composite prototype TCAD tool to predict (1)BMD distribution, (2)gettering profiles, and (3)stress/slip behavior based on process sequences prior to real device fabrication. Herein, we report on (i)system diagram and basic algorithm of a prototype composite tool, (ii)marked BMD radius distributions in terms of process sequences and initial resolved [O_i] concentrations, (iii)Fe and Cu gettering characteristics for BMD and in boron buried regions. Also, we discuss thermal budget criteria, taking into account metal gettering efficiency for device reliability and process induced defect control in conjunction with S/D and channel impurity profiles.

2 General concept and models

A block diagram and basic algorithms of our composite prototype system are presented in Fig.1. In the BMD part, oxygen precipitation characteristics were calculated based on the Fokker-Planck model[2,3] presented by eq(1). Oxygen diffusion caused by BMD growth and Gibbs free energy for BMD grain were coupled and solved at each time step using eq(2). BMD radius and distribution data were fed into the gettering simulation part. In RTP, a wafer surface would be irradiated by lamp ray and huge mechanical stress would be induced. Transient heat transport and deformation/balance were solved in the slip/stress module under a boundary condition of fixed temperature of top surface and heat sinks of tri/quadric-supporting points. Figure 2 illustrates mesh structure, models implemented and execution areas for BMD, gettering, and thermal stress/slip calculation parts. Material coefficients for diffusivity, solid solubility, reaction rates etc. were checked and customized in the tool using experimental values[4,5].

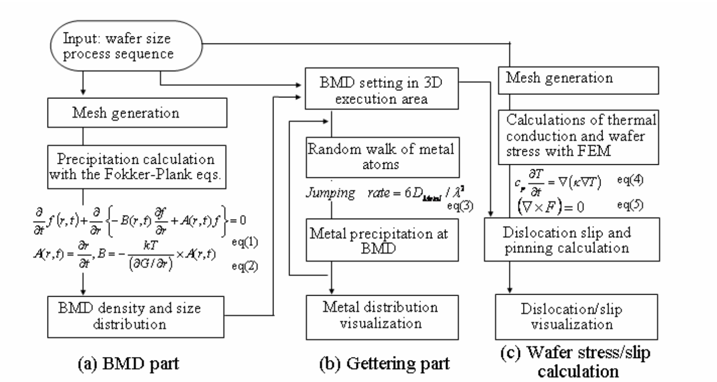

Figure 1: System diagram of wafer processing tool. (a)r is a BMD radius, f(z,t) a size distribution function and G Gibbs free energy. (b)Metal atoms are treated as particles. (c)T, κ and F are temperature, thermal conductivity and force.

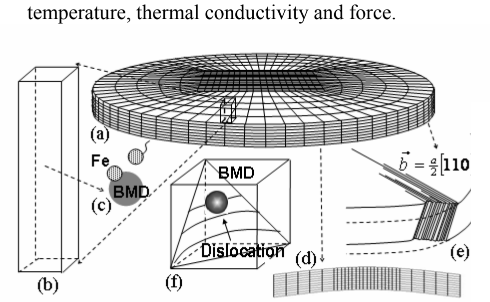

Figure 2: Schematic illustrations of mesh structure, models implemented and execution areas. (a)Wafer mesh, (b)area of BMD execution, (c)gettering model concept, (d)thermal stress calculation, (e)generation of slip, and (f)model for dislocation pinning with BMD.

3 Simulated results and discussions

Since the oxygen profile remains one of the key issues in the determination of substrate stiffness and BMD/gettering efficiency behaviors from the view-point of industry, we applied our prototype tool to these tasks. As an example, simulated results of interstitial oxygen concentrations through a typical process sequence for various initial [O_i] are shown in Fig.3. It should be noted in Fig.3(a) that [O_i] concentrations in substrates are found to have a complicated dependence on both initial [O_i] concentrations and thermal process sequences beyond our intuitive understanding. Typical results of radius distribution of BMD are shown in Fig.3(c). Based on an assumption that values deviated from initial [O_i] concentration correspond to precipitated BMD, we compared simulated BMD distribution/profiles with experimental data as shown in Figs.5 and 6 for our tool validations.

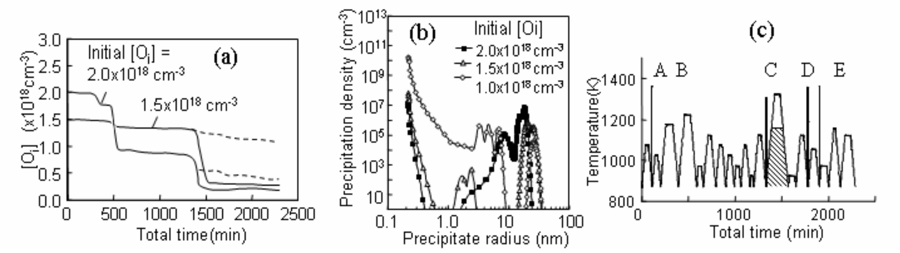

Figure 3: (a) Simulated results of [Oi] concentration as a function of process sequence for various initial [Oi] concentrations. (b) Radius distribution of BMD. (c) Typical input process sequence of scaled devices which we have simulated and done on experiments.

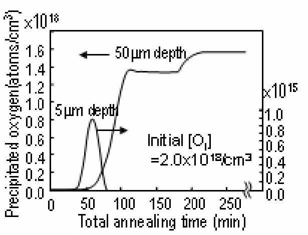

Figure4: Simulation results of oxygen precipitation for various regions.

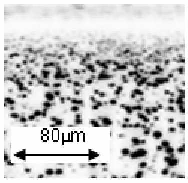

Figure 5: Experimental result of IR tomography. Dots present BMD.

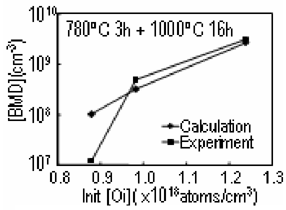

Figure 6: Simulated results of BMD density.

In order to maintain sufficient stiffness of wafers and to suppress dislocation slips, we have to optimize BMD radius distribution and profiles. We investigated process sequences. Broken lines in Fig.3(a) show results of optimized [O$_i$] concentration for sufficient stiffness based on the revised process sequence at a temperature indicated by 'C' in the figure, which was an annealing process of STI filling materials prior to making active regions.

We investigated Fe and Cu gettering characteristics in terms of BMD size/distribution and variation of boron profiles. As typical examples of output results, characteristic behaviors during cyclic heat treatment are shown in Figs 7, 8, and 9. It can be seen that Fe metals are mostly captured at BMD sites. Moreover, using animation, random diffusion motion of free Fe atoms and progress of precipitation can be seen. Cu gettering at the boron-doped area was simulated as shown in Fig. 9. Since solid solubility of Cu is very high in the boron-doped region, only a small part of Cu atoms are captured at BMD sites. It can be visualized that Cu atoms gather in the boron-doped region at R.T. and disperse after elevating the temperature to 200 ºC in a flash.

Slip generation during thermal process is another important issue requiring special attention in LSI process, otherwise patterns printed on the wafer would be distorted, and eventually device yielding would be reduced. We investigated temperature profiles, stress distribution, and deformation during typical RTP as shown in Figs. 10 and 11. Although this is still a prototype wafer processing tool, the simulated dislocation patterns shown in Fig.11 (a) agree well with the experimental results in Fig.11(b). It was found that BMD density in three dimensional space is

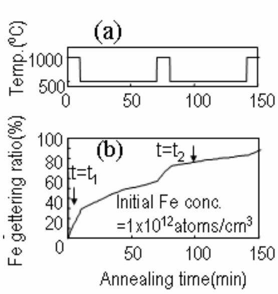

Figure 7: Typical output result of Fe gettering.

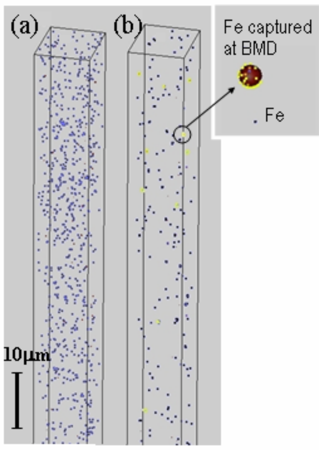

Figure 8: Snapshots of Fe gettering simulation. Fe distributions at t=t$_1$ and t=t$_2$ in Fig. 8 are shown in (a) and (b). Execution area is 10x10x300μm.

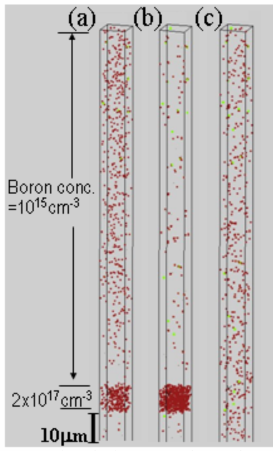

Figure 9: Simulation results of Cu diffusion and gettering characteristics. (a)Initail and (b)60min after at R.T. (c)Snapshot after elevating temperature from R.T. to 200 ºC. Cu atoms are captured partly at BMD sites.

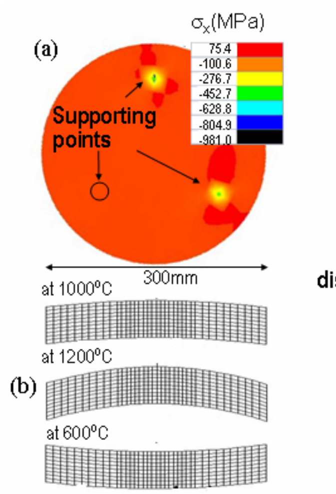

Figure10: Simulation results of (a)stress distribution and (b)distortion for 300mm wafer during typical FLA process.

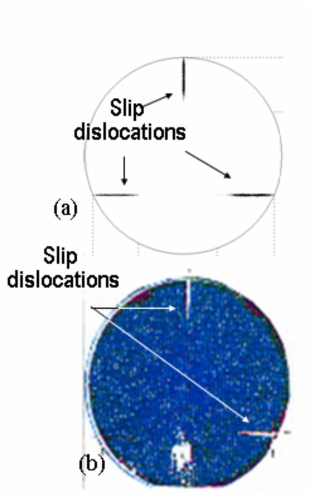

Figure11: (a) Dislocation slip simulation during an RTP. For simplicity, slip lines are modeled to be generated at supporting points and to be moved in stress field. Slip lines grow up until meeting BMD. (b)Experimental result of slip patterns on a wafer.

particularly important parameter in order to suppress slip sliding in prior to annealing time.

4 Summary

We developed a new prototype TCAD tool for wafer processing, particularly to predict BMD distribution, metal gettering characteristics, stress/slip dynamics from the view-points of industry such as reliability, reproducibility and cost reduction. We demonstrated through simulated results and experimental results that oxygen profiles and BMD distribution are key issues for wafer processing that are definitely interlinked with substrate stiffness, slip tolerances, and metal gettering efficiency. We also reported tool verification.

Acknowledgements

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