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On the Nucleation of Dislocations at Thin Film Edges on Silicon Substrates

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A theoretical model is developed which predicts the type of film edge induced defects in silicon substrates as a function of the film and substrate orientation. The obtained results are illustrated with high voltage transmission electron microscopy (HVEM) observations of defects in local oxidation (LOCOS) structures on (001) silicon substrates. Including the influence of intrinsic point defects on the homogeneous dislocation nucleation allows to derive a general expression for the temperature and time dependence of the critical film thickness resulting in defect generation.

1. Introduction

The fabrication of integrated circuits involves the use of several thin films either grown or deposited on the silicon substrate. The differences in film structure introduce large interface stresses which accumulate at the film edges. During subsequent high temperature treatments these stresses can become large enough either to activate latent dislocation sources or even to nucleate dislocations homogeneously. Extensive reports are available on the defect generation at nitride film edges [1-6], but little information exists for polysilicon/SiO_2 [7] or for silicon oxide films.[8]

A theoretical model, which predicts on geometrical grounds (film and substrate orientation) the type of nucleated defect (its Burgers vector, glide plane and equilibrium shape) [9], has been developed and succesfully applied to explain the defect configurations observed at nitride film edges after local oxidation processes.[9-10] The present paper gives a brief overview of the high voltage transmission electron microscope (HVEM) observations in (001) silicon substrates and discusses an extension of the model resulting in a general expression for the critical film thickness required for homogeneous dislocation nucleation. Important conclusions can be drawn with respect to the use of high oxygen content wafers for intrinsic gettering purposes. The difference in yield stress between floating zone (FZ) and Czochralski (CZ) material can be explained quantitatively.

HVEM observations

Along <110> edges 60° dislocations are often observed originating from cross glide of small half loops nucleated homogeneously at the edge (Fig. 1). An example of dislocation generation by the capture at the film edge of dislocations from external sources and subsequent growth and/or multiplication is represented in Fig.2a. The T(riangular) H(alf) L(oops) observed along <100> edges result from the capture of small prismatic loops punched out deeper in the bulk by SiO_x precipitates.[5] The prismatic nuclei are captured at the film edge by the stress field, transform in small THL's and while growing by glide are subsequently repelled towards the opposite edge (Fig.2d). An extensive review on HVEM observations of defect control in the local oxidation technology was recently reported elsewhere [6].

Theoretical nucleation model

1. Nucleation mechanism

The homogeneous dislocation nucleation can be described by a two step mechanism : first a small planar agglomerate of silicon self interstitials e.g. at an irregularity of the film edge, grows by climb and subsequently when the critical radius for dislocation glide is exceeded, growth by glide takes over until the equilibrium shape of the dislocation loop is reached. The heterogeneous

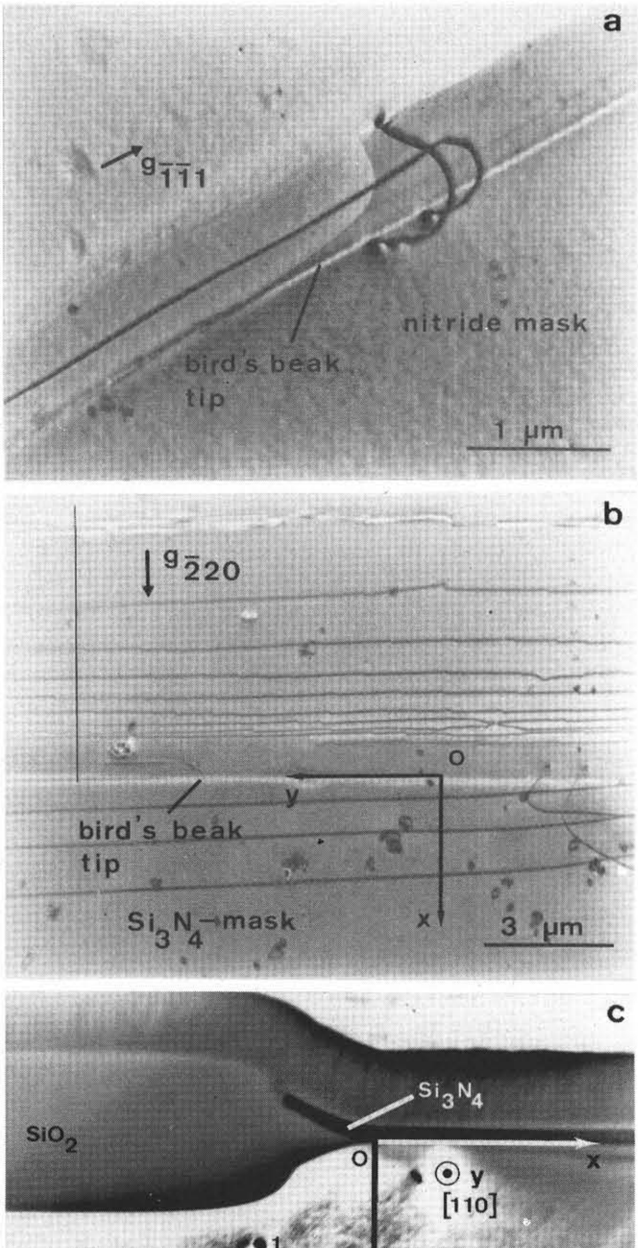

Fig. 1 (a) Plan view HVEM micrograph illustrating the generation of a 60° dislocation by cross glide of a "Hu" loop observed after a 10h wet oxidation at a [110] oriented 120 nm thick nitride film deposited straight on the silicon surface. (b) Plan view image showing a pile up of 60° dislocations in the stress field at the nitride film edge of (a). (c) Cross section micrograph of the same LOCOS structure. The piled up dislocations seen end on lie in close neighbouring (111) glide planes.

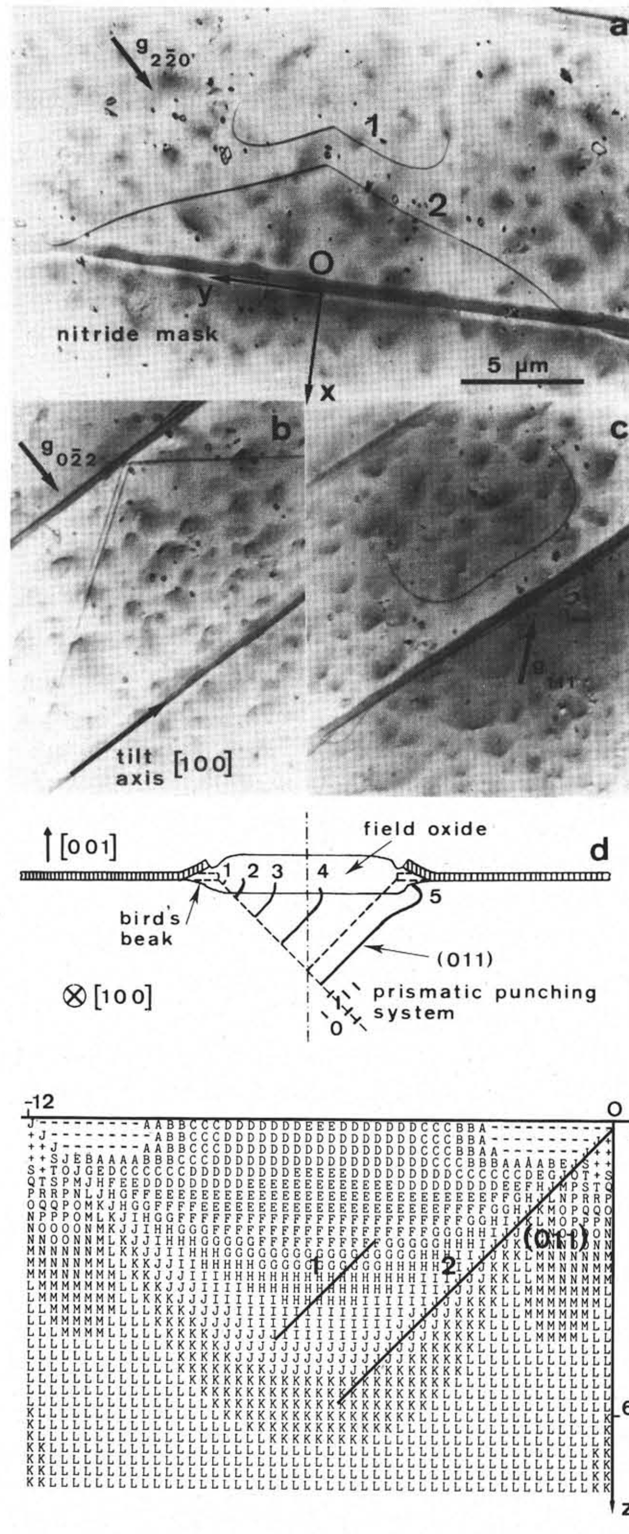

Fig. 2 Pair of triangular loops (THL's) (b = 1/2[011]) lying in (011) planes as observed in (c) which is obtained after tilting the specimen over 45° around the [100] tilt axis. Tilting the specimen 90° in the opposite direction, thus bringing the (011) plane horizontal shows that the THL's originate at the opposite film edge (b). A cross sectional view of the time sequence (0-5) of a growing THL is represented schematically in (d). (e) Cross section computer simulation of the external glide force F_D on a THL. The zero force is contained in interval J.

nucleation by the capture of dislocations from external sources and subsequent growth and/or multiplication can be described by considering the equilibrium of the internal and external glide forces.

2. Prediction of the type of defects[9])

The total climb force acting on a dislocation segment with Burgers vector $\bar{b}$ is the sum of the external and the internal climb forces :

$$F_n = F_{ne} + F_{ni} \qquad (1)$$

with $F_{ne} = \beta_{ij} b_i \beta_{\ell k} b_\ell \tau_{ij}$ (summation convention)

$\beta_{\ell k}$: the directional cosines between the coordinate system associated with the film structure and the crystallographic coordinate system

τ_{kj} : the stress components in the substrate

$F_{ni} = \frac{bkT}{\phi \ell^3} \ell n \frac{C_I}{C_I^*}$

C_I and C_I^* respectively the actual and the thermal equilibrium silicon self interstitial concentration

ϕ a constant which depends on the crystal structure (for Si $\phi \approx 1$) and ℓ the inter-atomic spacing.

When the minimal radius of curvature of the nucleus loop exceeds a critical value, growth by glide takes over until the equilibrium is reached between the external glide force F_p, and the counteracting line tension force F_ℓ and frictional force F_c :

$$\bar{F}_p + \bar{F}_\ell + \bar{F}_c = 0 \qquad (2)$$

with $F_p = \beta_{ij} n_i \beta_{\ell k} b_\ell \tau_{kj}$

n_i : the components of the unit vector perpendicular to the glide plane.

For the same type of Burgers vector, e.g. a/2<110>, only F_{ne} and F_p depend on the exact orientation of $\bar{b}$. Thus one can deduce the following nucleation criterion : the dislocations with a Burgers vector maximizing both F_{ne} and F_p will nucleate first. Their equilibrium shape is determined by solving equation (2) which can also be used to describe the capture and growth of dislocations from external sources (Fig. 2e).

3. Yield stress

3.1. Critical film thickness

For an inert anneal of FZ material the internal climb force is neglectable or $F_{ni} \approx 0$ and (1) reduces to $F_n = F_{nFZ}^{i(nert)}$. In general (1) can thus be rewritten as :

$$F_{ne} = F_{nFZ}^{i} - F_{ni}$$

As for temperatures above 600°C the critical glide force and thus also the critical radius R_c depend little on the temperature, the change in yield stress for CZ material as a function of temperature and time is dominated by the change of F_{ni}. The dislocation nucleation will occur preferentially during cooling down. Indeed, due to their long lifetime, an oversaturation of Si interstitials increases drastically when cooling down from a temperature T_2 to T_1 (both > 600°C). One can write [11]) :

$$F_{ne}(T_2) = F_{nFZ}^{i} - \frac{bkT_1}{\phi \ell^3} \ell n [1 + \frac{\Delta C_I(T_2)}{C_I^*(T_1)}] \qquad (3)$$

Taking into account that the external climb and glide forces (F_{ne} and F_p) are proportional to the film thickness and that growth of a dislocation nucleus occurs when the critical radius R_c is reached, one can calculate an approximate expression for the critical film thickness h resulting in defect generation. Including the possibility of a non horizontal force making an angle of arctgα with the x-axis finally leads to [11]) :

$$h(T) = A - B \ell n \left[1 + \frac{\Delta C_I(T)}{C_I^*(T_1)}\right] \qquad (4)$$

$$\text{with } A = \frac{m\sqrt{3}\mu b}{2(1-\alpha)(1+\sqrt{2})(1-\nu)\sigma} \ell n \frac{R_c}{5b} (2+\nu)$$

$$B = \frac{2m\pi k R_c T_1}{(1-\alpha)(1+3/\sqrt{2})\phi \ell^3 \sigma}$$

and supposing a minimal radius of curvature in the point $-x=mR_c$, $z=mR_c$. μ and ν are respectively the shear modulus and the Poisson ratio.

3.2. Inert anneal of oxygen rich CZ material

During thermal treatments above 600°C, the interstitial oxygen which is present in supersaturation in most CZ silicon, precipitates. The number and size of the precipitate nuclei present before the anneal step completely determine the precipitation kinetics. An accurate knowledge of the interstitial oxygen content of the thermal history of the wafer (growth conditions, pretreatments) is therefore essential to be able to predict the time and temperature dependent evolution of the change in silicon self interstitial concentration ΔC_I resulting from the oxygen precipitation. In the calculation the following assumptions are made :

- the number of precipitate nuclei N with radius r has a distribution given by : $N=N_0(\exp\frac{r_0}{r} - 1)$, with N_0 the total number of nuclei and r_0 a constant.
- the spontaneous recombination of injected interstitials occurs with a time constant τ.
- the precipitation of the interstitial oxygen on the supercritical precipitate nuclei follows an exponential law with time constant τ_1.
- the change in interstitial oxygen content due to the dissolution of the subcritical precipitate nuclei follows an exponential law with time constant τ_2.

Under these conditions one can calculate ΔC_I as [11] :

$$\Delta C_I = E(e^{-\frac{t}{\tau_1}} - e^{-\frac{t}{\tau_2}}) - F(e^{-\frac{t}{\tau_2}} - e^{-\frac{t}{\tau}}) \qquad (5)$$

with $E = \frac{\tau\Upsilon}{\tau_1-\tau}(C-C^*+\frac{\varepsilon C\tau_1}{\tau_1-\tau_2})$

$$F = \frac{\Upsilon\varepsilon\tau\tau_2 C}{(\tau_2-\tau)(\tau_1-\tau_2)}$$

and Υ : the number of silicon interstitials created per precipitated oxygen atom (=0.587 for amorphous SiO_2)

C : the initial interstitial oxygen concentration

εC : the interstitial oxygen concentration increase which would result from an instantaneous dissolution of the subcritical nuclei

C^* : the oxygen solubility at the temperature T.

Substitution of (5) in (4) and comparison with experimental yield curves obtained e.g. from isochronal anneals at different temperatures [2] allows to determine the critical radius R_C for dislocation nucleation. Expression (4) then allows to predict the critical film thickness for CZ material with known oxygen content and precipitation parameters. The obtained theoretical results explain why FZ material is much more resistant against film edge induced defect generation than oxygen rich CZ material. This should be kept in mind when selecting high oxygen content material for its beneficial influence with respect to wafer warpage and for intrinsic gettering purposes. The creation of a denuded zone free of interstitial oxygen may be advantageous for the prevention of the nucleation of bulk defects (SF and prismatic punching systems) in the active region of the devices but one must be aware that the high mobility and long lifetime of the large number of silicon interstitials created deeper in the bulk causes an increased dislocation nucleation risk at the film edges.

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