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Mathematical Modeling of Amorphous Layers Growth by Low Energy Ion Implantation

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Abstract: In this study, a simple mathematical model has been developed for the description of amorphous layer growth by low ion energy implantation. The model concerns the lower and higher dose range. It has been assumed that the damage depth distribution can be approximated by a Gaussian. The thicknesses of the amorphous layer and voids film, obtained assuming multi-layer model, have been found in relation to the ion damage straggling and amorphization threshold. The model concept and the corresponding calculations are discussed in details.

Key words: Low energy ion implantation, amorphous layer growth, ion beam, damage distribution, mathematical modeling

INTRODUCTION

Some cleaning and etching processing techniques (Ryssel and Ruge, 1978; Vitkavage and Irene, 1988; Singh *et al*., 1983; Buckner *et al*., 1986) of semiconductors surfaces are based on low energy ion beam bombardment. The implantation into the crystalline material introduces radiation damage with increasing of ion doses until entire amorphous layer is formed.

Radiation damage theories are based on the assumption that a lattice atom struck by an energetic atom must receive an amount of energy to be displaced from its lattice site. Therefore, the deposited ion energy can be used as well as the number of the produced defects (Ryssel and Ruge, 1978). It is well know that the most used theory of ions transport in the matter is the LSS-Theory (Lindhard *et al*., 1963). According to this theory, the ion range has Gaussian distribution with projected range R_p and projected range straggling ΔR.

In the present study, a simple mathematical description of the amorphous layer growth by low energy ion implantation will be introduced. In the low-energy range, the damage is localized to a thin surface layer.

For a more detailed analysis of ion target-interactions, it is necessary to develop suitable multi-layer model that can be fitted to the experimental data (Hu *et al*., 1991; Miyazaki and Adachi, 1993; Feng *et al*., 1991; Gal *et al*., 1994; Akimov *et al*., 1994).

Zexian and Oechsner (2000) have developed an analytical model to describe the generation of concentration profiles in binary solids under low energy ion bombardment. The model accounts, in particular, for preferential sputtering and radiation enhanced particle transport in solid.

The model used here concerned the lower and the higher dose range. In the model, it will be assumed that the maximum of the damage depth distribution is located no far from the interface oxide/semiconductor and that the distribution can be approximated by a Gaussian. The value of the ion dose determines the kind of the buried damaged layer (below or above the amorphous threshold, voids) and its extent in the depth. By this, the damaged system oxide/substrate will be treated as:

- A 3-layer model in the low dose range
- A 4-layer model at higher ion doses

The extensions of the damaged regions can easily calculate from the Gaussian distribution. The mathematical description provides information about the amorphization dose, the critical energy density the state of the damage distribution.

MODEL CONCEPT

During ion implantation the concentration of the point defects increases as a result of atomic displacements by nuclear collisions above an accumulated critical energy density, these defects will relax into an amorphous state. The amorphization dose D_a can then be defined as the ion dose required to deposit the critical energy density. This will be equivalent to the

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first appearance of an amorphous layer. The expression of the amorphization dose is given by:

$$D_a = \frac{2E_d N}{\left(\frac{dE}{dx}\right)_n} \quad (1)$$

where, N is the atomic density, E_d is the displacement Energy and $(dE/dx)_n$ is the nuclear stopping power of the ion. Because of homogeneous defect nucleation, the process mentioned first is well described by the critical energy density. This quantity indicates that energy density which has to be deposited in the target by the incoming ions so that the point defects accumulated turn into the amorphous state. It was shown in (Koprinarov *et al*., 1996, 1997) that the critical energy density C_a is given by:

$$C_a = D_a \left(\frac{dE}{dx}\right)_n \quad (2)$$

The damaged region is assumed as homogeneous layer with the multi-layer system oxide/damaged layer/substrate. Firstly, it will be assumed that the maximum of the damage depth distribution is located not far from the interface oxide/substrate and the distribution can be approximated by a Gaussian (Fig. 1).

This leads to the mathematical description of the energy distribution G(x):

$$G(x) = \frac{f(E)ED}{\sqrt{2\pi}\Delta R} \exp\left[-\frac{1}{2}\frac{(x-k)^2}{\Delta R^2}\right] \quad (3)$$

Here, E is the ion impact energy, x is the depth in the substrate, k is the shift of the distribution related to the interface ΔR is the straggling of the damage distribution. The approximation of the damage distribution by Gaussian is quite good, because only the part in the semiconductor must be considered, attributed to the missing influence of ion bombardment in the oxide. With increasing ion dose, the energy density reach the critical energy density C_a in the depth $x = k$. In Fig. 2, the dependence of G(x) on the ion dose is shown for the shifts $k<0$ and $k>0$. Above the amorphization dose, the thickness $\tilde{d}$ of the amorphous layer will be determined by $G(\tilde{d}) = C_a$ from the intersection point of the distribution G_3 in Fig. 2 with the C_a-line. From that, the thickness $\tilde{d}$ is simply given by the relation:

$$\tilde{d} = \sqrt{2\Delta R^2 \ln\frac{f(E)ED}{\sqrt{2\pi}\Delta R C_a}} + k \quad (4)$$

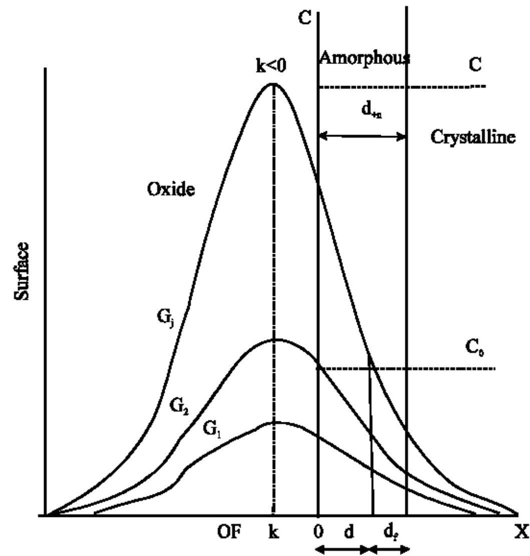

Fig. 1: Deposited Energy density distributions (Parameter: ion dose)

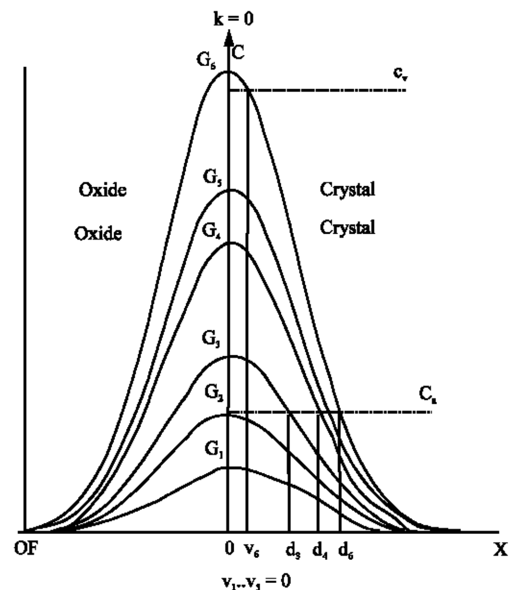

Fig. 2: Deposited Energy density in dependence on increasing ion dose (different regions of damage)

The relation (4) can further reduced to

$$\tilde{d} = \sqrt{2\Delta R^2 \ln\frac{D}{D_a}} + k \quad (5)$$

The amorphous layer is followed by the less damaged zone, which will be treated in the model in a rough approximation as an additional amorphous layer of the thickness d_f, here defined by:

$$d_f = \int_{\tilde{d}}^{\infty} \frac{D}{D_a} \exp\left[-\frac{1}{2}\frac{(x-k)^2}{\Delta R^2}\right] \quad (6)$$

That means, the residual damage distribution with an energy density per unit area given by the integral will be replaced by an equivalent amorphous zone with the same energy density per area $C_a \times d_f$. So, both layers are treated as one homogeneous amorphous layer with a thickness d_{eff} which will grow with the ion dose D:

$$d_{eff}(D) = \begin{cases} d_f & : \tilde{d} \le 0 \\ \tilde{d} + d_f & : \tilde{d} > 0 \end{cases} \quad (7)$$

Now, the 3-layer model is build up by the following layers:

Oxide/amorphous layer (d_{eff} (D))/substrate

As shown in Fig. 2, above an energy density C_v at the corresponding dose D_x the formation of voids is assumed (Ryssel and Ruge, 1978). Then, the homogeneity of the amorphous layer is disturbed and the 3-layer model cannot be used in this dose range. This leads to the mathematical description of the dose D_v:

$$\tilde{D}_v = D_v \exp\frac{k^2}{2\Delta R^2} \quad (8)$$

The thickness $\tilde{v}$ of the new layer (voids+amorph) can be deduced like the thickness $\tilde{d}$ taking into consideration the relation:

$$D_v = \frac{\sqrt{2\pi}\Delta R C_v}{f(E)E} \quad (9)$$

For high ion doses $D > D_v$, the thickness of the new layer (voids+amorph) is assumed to be:

$$\tilde{v}(D) = \sqrt{2\Delta R^2 \ln\frac{D}{D_v}} + k \quad (10)$$

Therefore, a 4-layer model is formed consisting of:

Oxide/voids+amorphous layer ($\tilde{v}$ (*D*))/amorphous layer (d_{eff} (D))/substrate.

RESULTS

In Fig. 3, the dependence of d_{eff}, $\tilde{d}$ and d_f on the ion dose is shown. For low ion doses with $D/D_a<1$ the thickness of the amorphous layer is zero and therefore

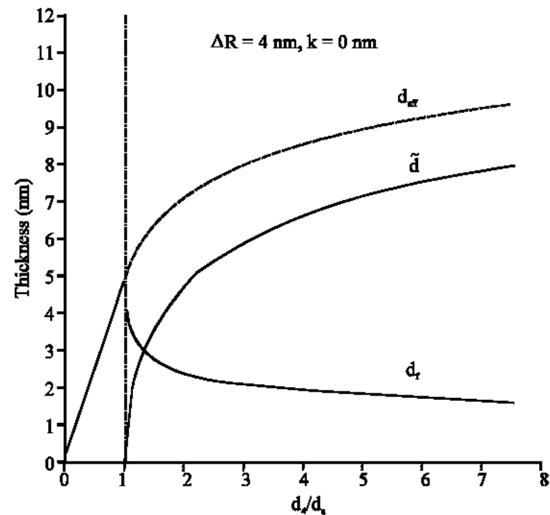

Fig. 3: Calculated d_{eff}, $\tilde{d}$ and d_f curves for ΔR = 4 nm and k = 0

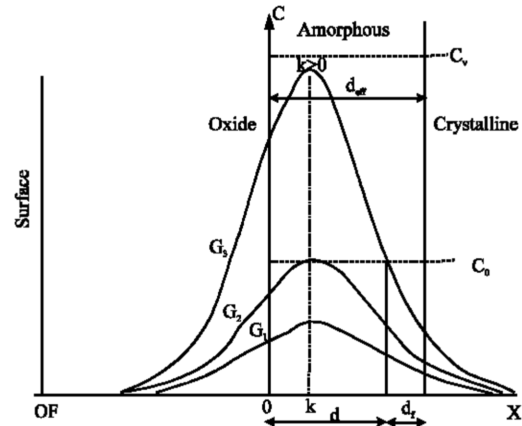

Fig. 4: Calculated curve pairs (d_{eff}, $\tilde{d}$) as function of ion dose for two values of ΔR (2 and 4 nm) the distribution shift k (+1 nm and -1 nm)

$d_{eff} = d_f$. For these doses the approximation is expected to be rather poor. Above the amorphization threshold, an increasing ion dose yields an increasing $\tilde{d}$ and a decreasing d_f. The amorphization fluence increase with decreasing ion impact energy; this variation is most pronounced for energies below 500 eV (Bock *et al*., 1993).

Therefore, the quality of the approximation improves rapidly with the growing ion dose. At D/D_a = 1 the corresponding d_{eff} curve shows a typical discontinuity in the slope. This point indicates precisely the appearance of the amorphous zone and in principle; D_a could be directly derived from experimental values.

So far, the maximum of the damage distribution has been assumed to be located in the interface

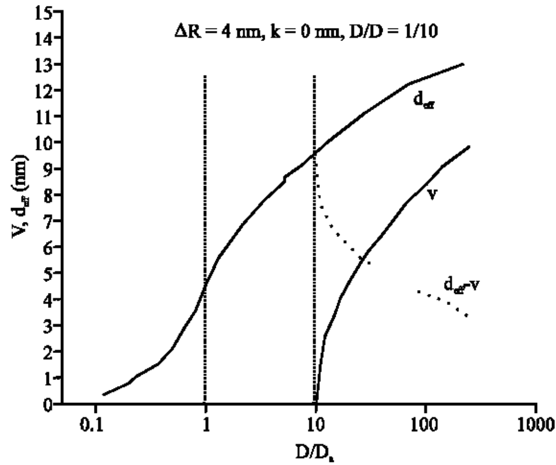

Fig. 5: Thicknesses, d_{eff} and $\tilde{v}$, of amorphous layer and voids respectively in dependence of D/D_a, calculated for ΔR = 4 nm und k = 0 nm

oxide/substrate. Normally, this can not be expected in the implantation procedure because the position of the damage distribution depends on the chosen ion energy.

Since there occurs a shift k of the damage distribution towards the semiconductor substrate, k must be added to $\tilde{d}$ or subtracted. In the case of a shift in direction of the surface.

In Fig. 4, two calculated curve pairs (d_{eff}, $\tilde{d}$) as function of ion dose are plotted for two hypothetic values of ΔR (2 and 4 nm) with distribution shift k (+1 nm and -1 nm).

As can be seen in Fig. 5, the extensions of the damaged layers can easily be calculated according to the 4-layer model. The dependence of the voids thickness $\tilde{v}$ on the ion dose is shown in logarithmic plot together with the amorphous layer thickness d_{eff}. The formation of voids is marked by the decrease of the quantity d_{eff}- $\tilde{v}$ (dashed line) and takes place above the dose D_v corresponding to the value $D_v = 10D_a$.

CONCLUSION

It was the main goal of the mathematical modeling to describe the growth of the damaged layer in the crystal for low and high ion doses. The information about relevant parameters as: amorphization dose, critical energy density the damage depth, have been provided using 3-layer model. According to the 4-layer model, above a threshold dose the formation of voids is assumed. The zone containing voids is extended in relation to the void-free damaged region.

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