ROLE OF LOCAL TEMPERATURE ON FORMATION OF AS-IMPLANTED DEFECTS

J. Gyulai', F. Pászti[2], E. Szilágyl[2] , N. Q. Khanh[1]

'KFKI Res. Inst. for Material. Sci., POB 49, H-1525 Budapest, Hungary
[2]KFKI Res. Inst. for Part. and Nuclear Phys., POB 49, H-1 525 Budapest, Hungary

ABSTRACT

The role of local temperature around a cascade is demonstrated. Calculations show that temperature dependence of heat conductivity has a major influence on types of primary defects. This, in turn, influences thermal path to arrive an annealed structure.
Experimental evidence will be given of this effect, say, by implantation into silicon of different thickness. Correlation is presented between bulk thermal properties of six different semiconductors and the critical temperatures separating Ion Beam Induced Epitaxial Crystallization (IBIEC) and Amorphization (IBIA).

1. INTRODUCTION

Together with other techniques critical in the production of modem electronic devices, ion implantation faces a constant challenge to meet growing requirements. E.g., for gate oxidation for the 0,18 μm and the 0.07 μm technologies of the coming years, the oxide thickness of CMOS transistor is 3 to 5 ± 0.2 nm, while the lattice spacing is 0.5 nm. Furthermore, these single atomic steps must not occur more often than at every thousandth surface atom, as a consequence of the density of tolerable surface states (l0^{9} cm^{-2}).
Most ULSI processing steps, however, bear one certain advantage over ion implantation. Namely, ion implantation is doubly effected by statistics.
First, the impact is random, second, processes within the cascade are statistical. The first problem will stay with us, but the second one can be handled to a certain extent by methods of "defect engineering". Thus, to keep direct ion implantation in business, the deepest microscopic understanding of the processes is needed. In this paper, we will stress the importance of precise control of the as-implanted defect state by thermal means to reach a proper final state. The following thermal treatment should produce functioning structure

* nearer to equilibrium state, but
* stable enough to avoid "aging", AE >> $k\,T$ (RT.)

A cascade-level understanding of processes is thus the only chance. to keep implantation in competition. It is to be remembered that new demands for miniaturization of devices, dopant redistribution during thermal treatments is detrimental.
To understand the problems let us review a microscopic picture of implantation

Table 1. Time scale of the scenario of implantation

Time, s BANG!	Event	Overlap by next ion
10^{-14}	Primary ion looses energy	
10^{-12}	Fast cascade develops	
10^{-10}	Slow cascade	
10^{-8}	Cooling	BANG! PIB LP[a]
10^{-6}	Frenkel pair diffusion	BANG! FIB Sp[2b]
10^{-4}	?	Dynamic annealing

Four theoretical approaches are coexisting to describe phenomena:

i) Monte Carlo type calculations (MC,[1,2]),
ii) Molecular- dynamics (MD, [3,4]),
iii) spike theories [SI,
iv) thermodynamic Miedema-type approach [6].

The MC description means TRIM and related codes, which describes kinetics of ranges and of defects, but has no feeling of chemistry, thus cannot account for lattice location. The molecular dynamics (MD) calculations are very realistic but still unrealistic in everyday praxis. MD methods clear up, however, basic events and point out directions for experiments and production praxis.
The spike theories are detailed, the events are well understood for ion beam mixing of metallic layers and at low temperature. lt. was shown that spike and radiation enhanced diffusion, RED, effects can overcome ballistic effects. Often even melting is experienced. For silicon there are basic differences:

- implants are done at $T_{imp} \geq$ room temperature (RT.),
- Si is a covalent crystal,
- its heat conductivity (κ) is excellent, but strongly decreases with T.

[a] Implantation with Pulsed Ion Beam, PIB, can involve melting over the sample surface and consequent Liquid Phase, LP, regrowth process because of active cascade overlap.
[b] For implantation with Focused Ion Beam, FIB, a delay cascade overlap occurs which allows dose rate-type effects similar to Solid Phase, SP, growth process.

In addition, processing brings in further complexity:

- native/process induced impurities can be present in Si, as well as
- mechanical stress,
- heat flow (wafer contact) and, for low energies, radiative cooling may occur,
- furthermore, already existing lateral structures influence heat conduction.

The pure thermodynamic treatment, the so-called Miedema-approach accounts for condition for substitutionality, etc., but cannot account for ranges and defect distributions.
The as-implanted wafer is then subjected to different treatments, which adds up to the total "thermal budget" of the process. To arrive at a proper final (secondary), possibly defect-free state, processing often termed as "Defect engineering" is used. This general term may involve thermal and athermal treatments, even introduction of certain additional defects to provoke proper defect reactions.
In this paper, as a consequence of temperature dependence of heat conduction, we would like to call attention on the importance of wafer temperature and of temperature of the near-the-cascade area.
Primary defect formation involves:

- Processes in a single cascade and in simultaneous and/or overlapping sub cascades,
- Superposition (maybe synergism) of processes, "active" zones.

Although effects of "light" and "heavy" ions (for the whole range of energies) are very much different locally, the extra energy (heat) deposited in that microscopic region will mostly be taken away by heat conduction.
Here, a correlation between thermal scenarios is suggested:

i) early findings for resolidification after a laser pulse [71, and of
ii) Ion Beam Induced Epitaxy (IBIEC) / Amorphization (IBIA) [8-lO].

For the first, it was found that a critical resolidification velocity, v_{crit} of approx. 20 m/s separates the crystalline ($v < v_{crit}$) and amorphous regrowth of silicon after a Q-switched laser pulse. This velocity roughly corresponds to 10^{-12}-10^{-11}s time to grow one atomic layer. This time scale is identical with that of the fast cascade [11].
Furthermore, from theories of the IBIEC/IBIA, a critical wafer temperature, T_{crit} can be defined which separates epitaxial growth from amorphization by the beam. In this paper, these two ideas will be applied to volumes around individual cascades. i.e., we assume that the same, v_{crit} resolidification velocity separates regimes of crystalline vs. amorphous regrowth in the cascade volume and the process is governed by T_{crit}, of the material-ion pair.
A simple heat conductivity theory for instantaneous source [12] suggests that the temperature profile contains κt in product, i.e.,

$$T(R,t)\,\alpha \left(\frac{1}{\kappa t}\right)^{3/2} \exp\left(\frac{-R^2}{4\kappa t}\right)$$

Thus, a decrease in heat conductivity, κ, around the cascade region allows a correspondingly longer time period, t, for the formation of the same isotherms. (R is the spatial coordinate.) This favors conditions for dynamic annealing, and vice versa.
In a previous paper [13], we called attention on the above correlating phenomena. The discussion given there will be briefly resumed.

2. MICROSCOPIC PICTURE AND DISCUSSION

We will neglect known or disputed details of cascade formation and decay (e.g., for light or heavy implant ions) by defining a volume (half sphere) which embraces a single cascade completely and will try to draw conclusions on the thermal state within when a strong dependence of thermal conductivity (κ) on temperature is taken into account.
If we consider the problem of heat conduction through this half sphere, around an individual cascade, the thermal energy flowing through the i-th and AR thick shell of the half-sphere at a radius R outside the cascade can be written as

$$T_i^{'} 2\pi R^2 \Delta t \kappa(T_i) =$$
$$(T_i^{'} + T_i^{''}\Delta R) 2\pi (R+\Delta R)^2 \Delta t \kappa(T_i^{'} + T_i^{''}\Delta R)$$

where T, , T,', and T_i'' are the temperature, its first and second derivative at the i-th shell and At is the corresponding infinitesimal time interval. In [13l, it was taken , $\kappa(T) = \kappa_0/T^n$, with n = 2. Furthermore, if the ambient temperature surrounding this sphere is equal with the critical temperature separating IBIEC and IBIA for a given material-ion pair, T_{crit}, (measured value) and we denote the melting temperature with T_m and define R_0 as the spatial coordinate of the solid-liquid interface, where $T = T_m$, we arrive at the solution for the thermal balance between the heat at melting and the heat transport through the half-sphere

$$(T_m - T_{crit})T_m / T_{crit} = R_0 v \rho \Delta H / \kappa_m$$

Here ρ is the density, ΔH is melting enthalpy, and κ_m. denotes the value of the heat conductivity at melting temperature.

It was shown in [13] that using measured data from the literature [141, in this case for six different semiconductors, Si, Ge, GaP, InP, GaAs, and lnAs, a correlation of the criti-

cal temperature and materials properties at melting temperature can be gained. The result can be seen in Fig. 1. The correlation is reasonable enough to show that this simple theory points on an important factor governing regrowth after cascade activity. The slope of the fitting line equals O.021 KslCM2 . This value gives *vR.* in the model. As quoted above [71, the critical resolidification velocity for Si is - 20 mls. It is very comforting for a crude model like this that this v-value gives R,, - O.1 gm, which is about the expected order of magnitude. The Figure can predict hitherto unmeasured values of *T,,,,* e.g., for SiC around l4OO'C.

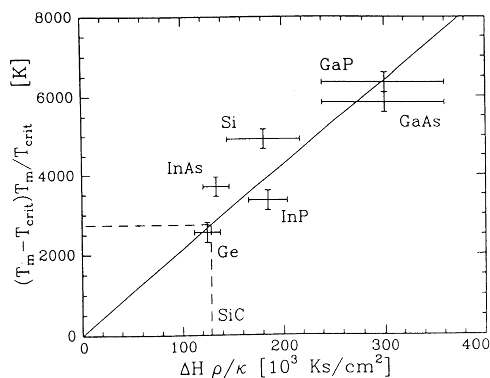

Figure 1- Correlation between characteristic temperatures and melting enthalpy over heat conduction for individual cascades T_{crit} data for six different semiconductors were measured by Glaser et al [14]. Data predicted T_{crit} being around 1400°C.

In this concept, implantation temperature, T_{imp} influences primary defect state through its effect on the heat flow out from the cascade area. If this "quench rate"-type effect will be enhanced, say, by decreasing T_{imp} conditions for amorphization are favored, and *,vice versa.*

Furthermore, "hot implantation" controls (decreases) energy flux out from the cascade area *by influencing the thermal conductivity.* We believe that this is the mechanism how T_{imp}, influences the as-implanted defect state. We suggest a new way of thinking, stating that dramatic effects of implantation temperature on dynamic annealing are mainly connected to changes in κ(7) and in gradient T'.

Analysis showed that as R_0 decreases in time during the resolidification process, ν must continuously increase.

Thus, there is a marginal size of the still molten zone, where ν passes the velocity separating crystalline from amorphous regrowth. Therefore, at the end of the resolidification, at least a small disorder region will always form.

To demonstrate the eventual effect of local temperature in silicon, the following experiment was made. Etch pits were made into originally 450 µm thick silicon wafers using a diamond drill of 5 mm diameter followed by a chemical etch remove the mechanically damaged layer. The thinnest membranes left were about 55 µm thick, These wafers were then implanted in an Extrion 350 D implanter supplied with a Wayflow end station with sub-amorphizing dose of 100 keV argon

Dose rates were ~80 nA/cm. The primary defect structure was analyzed Rutherford backscattering and channeling with extreme low analyzing beam current to avoid annealing during measurements (Fig. 2).

Measured damage distributions showed slightly enhanced dynamic annealing for the thin portion of the wafer having somewhat reduced heat transfer as a consequence of the shorter distance between the cascade region and the thermal bridge between the back side of the wafer and the heat sink.

We feel these findings comforting in a sense that for practical implantations with low dose rates the decrease in heat transfer does not have a substantial effect on dynamic annealing, i.e., on the distribution of primary defects. In future experiments, we are planning to control the model for higher dose rates and for heavier projectiles, and for other semiconductors than silicon, too.

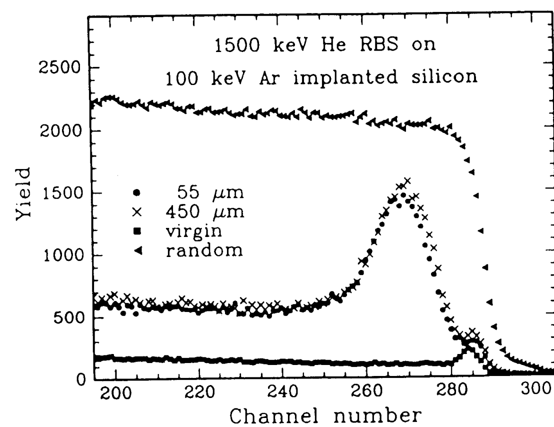

Figure 2 - Comparison between as-implanted defect structures of Si of different thicknesses after implantation with 100 keV, 1.8 x 10^{14} ion/cm^2 argon ions. Note the slight difference in dynamic annealing attributed to difference of the heat transfer bridge between the original and thinned wafer.

Furthermore, the importance of local, microscopic temperature conditions governed by details of sample cooling are essential in setting the primary defect states and, thus, annealing of the dopants.

We believe that often inconsistent studies of dopant annealing found in the literature can possibly be explained by the different thermal conditions, thus different as-implanted defect states, in different end stations of the implanters. This may even have led to the endless dispute, e.g., on usefulness of preamorphization, or on the superiority of BF@+ (preamorphization and) B+-ion implantation. lf this is true, it is easy to explain, why simulation programs for implantation need local experimental data as input.

It is obvious that the model implies dose rate effects, too. We suggest that poorer thermal diffusivity of III-V com-

pounds is, at least partially, responsible for dose rate effects even at regular implantation current densities.
In conclusion, importance and use of thermal balance during ion implantation was pointed out. Consequences on end chambers were presented.
A way of speaking was proposed, i.e., the dependence of local wafer temperature on heat transfer controls the rate of recombination of defects in the active cascades, thus the as-implanted defect state.
Similarly, implantation at different temperatures determines the as-implanted defect state through its influence on the heat transfer from the cascade area.

ACKNOWLEDGMENTS

The authors are indebted to numerous colleagues. Special thanks are due to coworkers of the Accelerator Laboratory at KFKI-RIPNP, especially, for a quick troubleshooting. Partial support came from OT'KA Grant #TO l7344, Hungary.

REFERENCES

1. e.g. J.P. Biersack and L.G. Haggmark, Nucl. Instr. Meth. 174 (l980) 257.
2. M. Posselt, Nucl. Instr. Meth., B 55 (l991) 676.
3. E.g. T. Diaz de Ia Rubia, R.S. Averback, R. Benedek, and H.Hsieh, J. Mat. Res., 4 (l989) 579.
4. F. Rossi and M. Nastasi, J. Appl. Phys., 69 (l991) 1310.
5. J.A. Davies: High Energy Density Collision Cascades and Spike Effects, in "Ion Implantation and Beam Processing" Eds. J.S.Williams and J.M.Poate, Acad. Press Australia, pp.81-99; G.H. Vineyard, Radiat. Eff., 29 (l976) 245; U.G. Akano, D.A. 'nompson, J.A. Davies, and W.W. Smeltzer, J. Mater. Res. 3 (l988) 1057; S-J. Kim, M-A. Nicolet, and R.S. Averback, Nucl. Instr. Meth. B 19120 (l987) 662; U.G. Akano, D.A. 'Rompson, W.W. Smeltzer, and J.A. Davies, J. Mater. Res. 3 (l988) 1063.
6. A.R. Miedema, Philips Tech. Rev., 36 (l976) 217; calculations for implants in Li, see E.N. Kaufman, R. Vianden, T.E. Jackinan, T.E. MacDonald, and L.G. Haggmark, J. Phys. F: Metal Phys 9. (l979) L23; for Si, see G. Odor and J. Gyulai, Nucl. Instr. Meth. B 30 (l988) 217.
7. A.G. Cullis, H.C. Webber, N.G. Chew, J.M. Poate, and P.Baeri, Phys. Rev. Lett., 49 (l982) 219.
8. G. Alestig, G. Holmen, and J. Linnros, J. Appl. Phys., 62 (l987) 409.
9. R.G. Elliman. D.C. Jacobson, J. Linnros, and J.M. Poate, Appl. Phys. Lett.. 51 (l987) 314.
10. R.G. Elliman, J.S. Williams, W.L. Brown, A. Leiberich, D.M. Maher, and R.V.Knoell, Nucl. Instr. Meth., B 19120 (l987) 435.
11. R. Kelly: Implantation, recoil implantation and sputtering, in "Ion bombardment modification of surfaces", 0. Auciello and R. Keily, eds. (Elsevier, Amsterdam, 1984), p. 44.
l2. H.S. Carslaw and J.C. Jaeger, Conduction of heat in solids (Clarendon Press, Oxford,1959)
I 31 J. Gyulai, F. Pászti, and E. Szilágyi, Nucl. Instr. Meth. B 106 (l996) 328.
l4. E. Glaser, P. Bachmann, E. Schultz, S. Schippel, and U. Richter, Nucl. Instr. Meth. B 106(1996)281.