Monte Carlo Simulation of Silicon Amorphization During Ion Implantation

W. Bohmayr*, A. Burenkov◇, J. Lorenz◇, H. Ryssel◇□, and S. Selberherr*

*) Institute for Microelectronics, TU Vienna, Gusshausstrasse 27-29, A-1040 Vienna, Austria
Phone +43/1/58801-3755, FAX +43/1/5059224, e-mail bohmayr@iue.tuwien.ac.at

◇) Fraunhofer-Institut für Integrierte Schaltungen-Bauelementetechnologie
Schottkystrasse 10, D-91058 Erlangen, Germany

□) Lehrstuhl für Elektronische Bauelemente, Universität Erlangen-Nürnberg,
Cauerstrasse 6, D-91058 Erlangen, Germany

When a sufficient high dose of energetic ions is implanted into a silicon crystal, irradiated zones of the crystal are transformed to an amorphous state. The thickness and spatial location of the amorphous layers determine the type of the extended defects and the number of point defects remaining in the silicon crystal after a recrystallization step. It is believed that the lateral diffusion of the defects is a possible source of the inverse short channel effect in MOS transistors. We present an accurate multi-dimensional model to predict the range of amorphous layers within ion implanted single-crystal silicon. The critical parameters ruling the amorphization process are the implantation dose D, the ion mass and energy, and the substrate temperature T which are all taken into account by our simulation method. The kinetic properties of amorphous silicon layers are well characterized [1] but the mechanisms of its formation by ion bombardment are still under investigation [2][3] and a quantitative description of this phenomenon within a TCAD environment was not available up to now.

The approach is based on a critical damage energy model [1] which assumes that the transformation to the amorphous state happens when the accumulated damage energy generated by ion beam exceeds a critical threshold. For example, the threshold damage energy E_C at low temperatures ($T \leq 82$K) for silicon self-implantation is about 12eV/atom [4]. The simplest approximation of a constant E_C would neglect the temperature and depth dependences of such amorphization processes [1]. The fundamental idea of our approach is the assumption that temperature dependent parameters are local functions of the deposited damage energy E_D (Fig. 1). In fact, E_D is a measure for the cascade density and areas with a lower density are assumed to anneal easier at a certain temperature compared to stronger damaged regions. Therefore we use (1) to model the temperature dependence of E_C and we use E_D and (2) to determine the depth dependence of each parameter in (1).

Using VISTA/MCIMPL [5] we calculated two-dimensional distributions of $^{28}Si^+$ ions implanted at 150keV and 300keV, with a dose of $3 \cdot 10^{14}$cm^{-2} through a 1.0μm wide window into (100) oriented single-crystal silicon covered by 1.0nm of oxide. The wafer was tilted by 7° in a (100)-type direction. First, we fitted the observed relation between E_C and T [1] at the depth of the damage-peak $E_{D,max}$ (cf. Fig. 1; $E_{D,max}$ = 25.2eV/Å/dose at 0.13μm for 150keV, $E_{D,max}$ = 21.7eV/Å/dose at 0.30μm for 300keV) by an analytical relation [1]. For every spatial location $\vec{r}$

$$E_C(T) = E_{C0} \cdot \left(1 - \exp\left(\frac{E_{ACT} \cdot (T - T_{INF})}{2kT \cdot T_{INF}}\right)\right)^{-2} \qquad (1)$$

energy	[keV]	150	300
E_{C0}	[eV/atom]	12	12
$E_{ACT,min}$	[meV]	120	120
$T_{INF,max}$	[K]	450	426

holds, where E_{C0} is the threshold damage energy at low temperature ($\leq$ 82K), E_{ACT} is the activation energy, k is Boltzmann's constant, and T_{INF} is the temperature above which one would need an infinite dose for amorphization (cf. Fig. 2). Secondly, the depth dependence of E_{ACT} and T_{INF} [1] is modeled by means of E_D and with the following power laws

$$T_{INF}(\vec{r}) = T_{INF,max} \cdot \left(\frac{E_D(\vec{r})}{E_{D,max}}\right)^{e_T} \quad E_{ACT}(\vec{r}) = E_{ACT,min} \cdot \left(\frac{E_{D,max}}{E_D(\vec{r})}\right)^{e_E} \qquad (2)$$

energy	[keV]	150	300
e_T	[1]	0.35	0.35
e_E	[1]	0.55	0.55

Further comparisons show that $E_{ACT,min}$ only slightly depends on the ion energy and that $T_{INF,max}$ can be scaled by $\frac{T_{INF,max,150keV}}{T_{INF,max,300keV}} = \left(\frac{E_{D,max,150keV}}{E_{D,max,300keV}}\right)^{e_T}$ (cf. Fig. 2). Combining (1) and (2) we get the damage energy $E_C = f(\vec{r})$ curves at a certain T (Fig. 3). We assume that E_D is independent of T and hence it is proportional to D. Fig. 4 shows the necessary implantation dose D to obtain amorphization at a given depth for several substrate temperatures T. The results are in good agreement with the experimental data [1].

To show the applicability of our new method we performed LDD and drain implantation simulations of a NMOS device (Fig. 5). A continuous amorphous layer is predicted by our model after the drain implant (Fig. 6) and the lateral extension of this layer is smaller than the one of the LDD region. Therefore more defects may survive the recrystallization step in this particular region.

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[5] W. Bohmayr et al., "Statistical Accuracy and CPU Time Characteristic of Three Trajectory Split Methods for Monte Carlo Simulation of Ion Implantation", *SISPAD*, Erlangen, Germany, pp. 492–495, 1995.

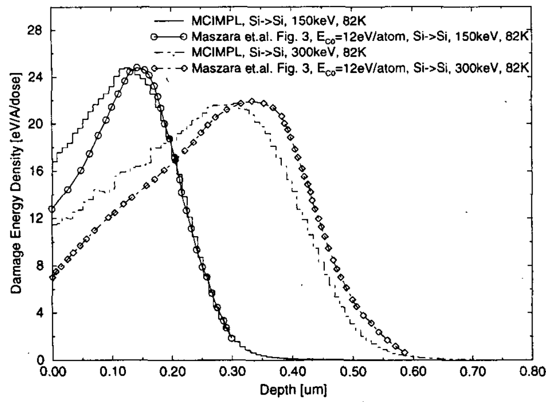

Figure 1: Deposited damage energy per Å and D vs. depth for 150keV and 300keV $^{28}Si^{+}$ ions implanted into crystalline silicon; comparison between MCIMPL simulations and experimental results at 82K [1].

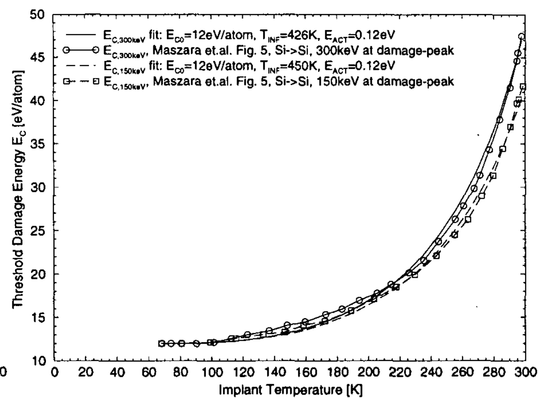

Figure 2: Threshold damage energy per atom vs. implant temperature for 150keV and 300keV implants; comparison between fitting function and experimental results at damage-peak [1].

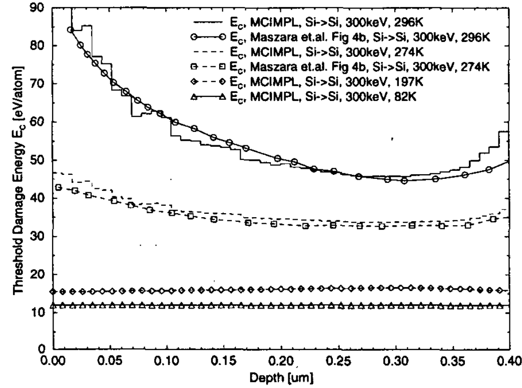

Figure 3: Threshold damage energy per atom for amorphization of silicon substrate with $^{28}Si^{+}$ ions vs. depth at which amorphous-crystalline transition is observed; comparison between MCIMPL simulations and experimental results at several temperatures [1].

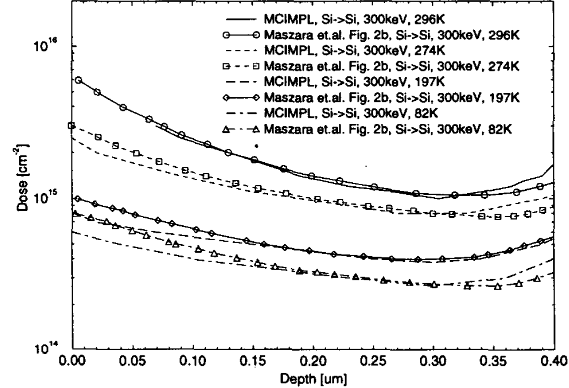

Figure 4: Threshold values of dose for which the crystalline silicon becomes amorphous vs. depth; comparison between MCIMPL simulations and experimental results at several temperatures [1].

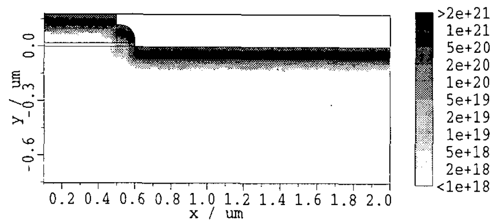

Figure 5: As-implanted profile of a typical two-dimensional technology-related example at T = 296K. First implantation step: $^{15}P^{+}$ ions, 30keV, $2 \cdot 10^{14}cm^{-2}$, 7° tilt; second implantation step: $^{33}As^{+}$ ions, 60keV, $5 \cdot 10^{15}cm^{-2}$, 7° tilt.

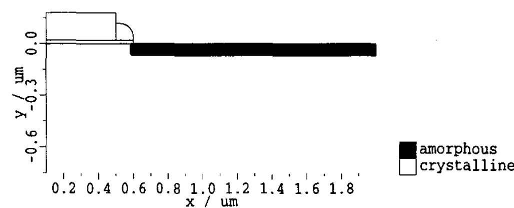

Figure 6: Resulting amorphous layer of our two-dimensional example calculated at T = 296K.

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