

A Calibrated Model for Silicon Self-Interstitial Cluster Formation and Dissolution

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Abstract—The formation and dissolution of Silicon self-interstitial clusters is linked to the phenomenon of TED (transient enhanced diffusion) which in turn has gained importance in the manufacturing of semiconductor devices. Based on theoretical considerations and measurements of the number of self-interstitial clusters during a thermal step we were interested in finding a suitable model for the formation and dissolution of self-interstitial clusters and extracting corresponding model parameters for two different technologies (i.e., material parameter sets). In order to automate the inverse modeling part a general optimization framework was used. Additional to solving this problem the same setup can solve a wide range of inverse modeling problems occurring in the domain of process simulation. Finally the results are discussed and compared with a previous model.

I. INTRODUCTION

The purpose of this work is to find a calibrated model for the formation and dissolution of Silicon self-interstitial clusters of {113} or {311} defects. A good calibrated model for self-interstitial clustering is important for accurately simulating the TED (transient enhanced diffusion) of impurities. TED is the fast displacement of impurities in the first thermal step just after implantation and the simulation of its evolution and magnitude is important in the manufacturing processes of submicron devices [1].

The source of the Silicon self-interstitials was shown to be the {113} defects which are rod like clusters of interstitials [2]. Counting the amount of self-interstitials is a non-trivial task: from transmission electron micrographs the number of interstitials in each defect and thus the total number has to be measured. In [3] one can find measurements giving the number of interstitials as a function of time for annealing at four temperatures (670°C, 705°C, 738°C, and 815°C) and $5 \cdot 10^{13} \text{ cm}^{-2}$, 40keV implants. These measurements are shown in detail in Figure 1 and provided the basis for this inverse modeling problem. For the computations we used TSUPREM-4 [4] and the optimization framework SIESTA [5], [6].

We were interested in finding solutions for two different technologies corresponding to different values of several TSUPREM-4 variables. In the following we will call these parameter sets the high and the low parameter set (the latter being the TSUPREM-4 default values).

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The parameters and their values are shown in Table I.

Since the rate of formation and dissolution is not yet fully understood, the model used contains several proposed models (e.g., [1]) as special cases [4]. After describing the model and the details of the inverse modeling problem we present the results and the calibrated model.

II. MODELING SILICON SELF-INTERSTITIAL CLUSTER FORMATION AND DISSOLUTION

In [1] the following equation describing interstitial cluster kinetics is given:

$$\frac{\partial C}{\partial t} = 4\pi\alpha a D_I I C - \frac{C D_I}{a^2} e^{-E_b/kT}, \quad (1)$$

where $D_I = D_0 e^{-E_m/kT}$ is the interstitial diffusivity, a is the average interatomic spacing, α is the capture radius expressed in units of a , $C(t, x)$ is the concentration of interstitials trapped in clusters, $I(t, x)$ is the concentration of free interstitials and T is the annealing temperature.

Here the main formula of the model for the change of the concentration of clustered interstitials is

$$\frac{\partial C}{\partial t} = K_{fi} \frac{I^{ifi}}{I_{*}^{isfi}} + K_{fc} \frac{I^{ifc}}{I_{*}^{isfc}} (C + \alpha I)^{cf} - K_r C^{cr}, \quad (2)$$

where $C(t, x)$ denotes the concentration of clustered interstitials, t time, $I(t, x)$ the concentration of unclustered interstitials.

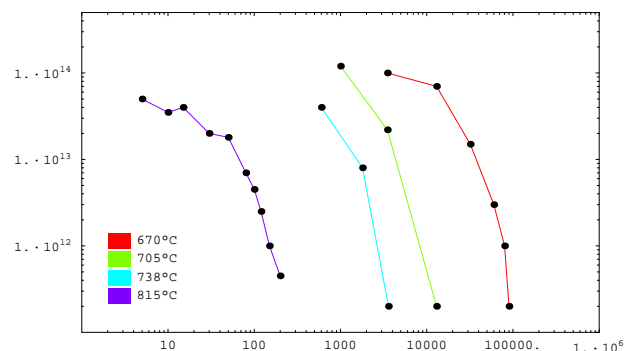


Fig. 1. The Silicon self-interstitial density (in cm^{-3}) as a function of time (in s) for different annealing temperatures (interstitials stored in {113} or {311} defects after $5 \cdot 10^{13} \text{ cm}^{-2}$, 40keV implants).

TSUPREM-4 variable	High Parameter Set	Low Parameter Set	Unit
interstitial mat=silicon cequil.0	$2.9 \cdot 10^{24}$	$1.25 \cdot 10^{29}$	cm^{-3}
interstitial mat=silicon cequil.E	3.18	3.26	eV
interstitial mat=silicon kb.0	$1.2 \cdot 10^{-5}$	$1.0 \cdot 10^{-21}$	cm^3s^{-1}
interstitial mat=silicon kb.E	1.77	-1.0	eV
interstitial silicon /oxide ksurf.0	$5.1 \cdot 10^7$	$1.4 \cdot 10^{-6}$	cm s^{-1}
interstitial silicon /oxide ksurf.E	1.77	-1.75	eV
vacancy mat=silicon d.0	$3.0 \cdot 10^{-2}$	$3.65 \cdot 10^{-4}$	cm^2s^{-1}
vacancy mat=silicon d.e	1.8	1.58	eV
vacancy mat=silicon cequil.0	$1.4 \cdot 10^{23}$	$1.25 \cdot 10^{29}$	cm^{-3}
vacancy mat=silicon cequil.E	2.0	3.26	eV

TABLE I
THE DIFFERENCES BETWEEN THE HIGH AND LOW (DEFAULTS) PARAMETER SET.

Variable	Interval	Unit
d0	[25, 1000]	cm^2s^{-1}
dE	[1.4, 1.85]	eV
kfi0	$[10^{20}, 10^{28}]$	$\text{cm}^{-3(1+\text{isfi}-\text{ifi})}\text{s}^{-1}$
kfiE	[3.4, 6.0]	eV
ifi	constant = 2	1
isfi	constant = 2	1
kfc0	$[10^{17}, 7 \cdot 10^{19}]$	$\text{cm}^{-3(1+\text{isfc}-\text{ifc}-\text{cf})}\text{s}^{-1}$
kfcE	[4.9, 5.2]	eV
ifc	constant = 1	1
isfc	constant = 1	1
α	[0, 5000]	1
cf	constant = 1	1
kr0	$[1.5 \cdot 10^{16}, 10^{18}]$	$\text{cm}^{-3(1-\text{cr})}\text{s}^{-1}$
krE	[3.0, 3.62]	eV
cr	constant = 1	1

TABLE II
VARIABLES, THEIR INTERVALS, AND THEIR UNITS.

tered interstitials, and $I_*(t, x)$ the equilibrium concentration of interstitials (which can be found by solving $\partial C(t, x)/\partial t = 0$). There is a number of parameters to be adjusted: K_{fi} , K_{fc} , K_{r} (the reaction constants); the exponents I^{ifi} , I^{isfi} , I^{ifc} , and I^{isfc} , cf, and cr; and finally α .

The reaction constants have the form

$$\begin{aligned} K_{\text{fi}} &= \text{kfi0} \cdot e^{-\text{kfiE}/kT}, \\ K_{\text{fc}} &= \text{kfc0} \cdot e^{-\text{kfcE}/kT}, \\ K_{\text{r}} &= \text{kr0} \cdot e^{-\text{krE}/kT}, \end{aligned}$$

with $\text{kfi0} > 0$, $\text{kfc0} > 0$, and $\text{kr0} > 0$. Here T is the temperature (in Kelvin) and $k = 8.617 \cdot 10^{-5} \text{eV} \cdot \text{K}^{-1}$ the Boltzmann constant. Since the coefficients kfi0 , kfc0 , and kr0 are positive, the first two terms in (2) are responsible for the formation of clusters and the last term for the dissolution. The sum of interstitials counted

High Parameter Set (mean relative error 0.389666):

Variable	SIESTA variable	Best point found
d0	d-0	51.7282
dE	d-e	1.76996
kfi0	kfi-0	$4.97576 \cdot 10^{24}$
kfiE	kfi-e	3.77408
kfc0	kfc-0	$4.36789 \cdot 10^{19}$
kfcE	kfc-e	4.95
α	kfc-i	1099.63
kr0	kr-0	$2.77935 \cdot 10^{16}$
krE	kr-e	3.56997

Low Parameter Set (mean relative error 0.504462):

Variable	SIESTA variable	Best point found
kfi0	kfi-0	$1.14156 \cdot 10^{25}$
kfiE	kfi-e	3.94079
kfc0	kfc-0	$1.5051 \cdot 10^{19}$
kfcE	kfc-e	5.81858
α	kfc-i	1563.1
cf	cf	1.01287
kr0	kr-0	$1.06467 \cdot 10^{17}$
krE	kr-e	3.84503
cr	cr	0.9639

TABLE III

RESULTS FOR THE HIGH AND LOW PARAMETER SETS WITH THE ABOVE FREE VARIABLES. THE MEAN RELATIVE ERROR FOUND IS 0.389666 FOR THE HIGH PARAMETER SET AND 0.504462 FOR THE LOW PARAMETER SET.

in C and I remains constant and the initial value of C is 10^9cm^{-3} .

The ratio I/I_* of the concentration of the unclustered interstitials and its equilibrium concentration is often called the interstitial supersaturation. Here additional exponents modify the interstitial supersaturation which appears in the form $I^{\text{ifi}}/I_*^{\text{isfi}}$ and $I^{\text{ifc}}/I_*^{\text{isfc}}$.

The first term $K_{\text{fi}}(I^{\text{ifi}}/I_*^{\text{isfi}})$ describes the joining of

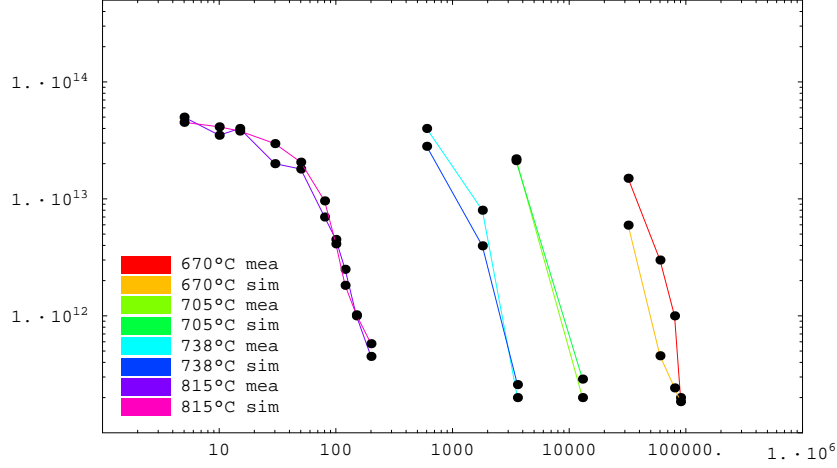


Fig. 2. Result for the high parameter set corresponding to parameter values shown in Table III. The logarithm (base 10) of the simulated and measured concentration [cm^{-3}] of interstitial clusters is shown depending on time [s].

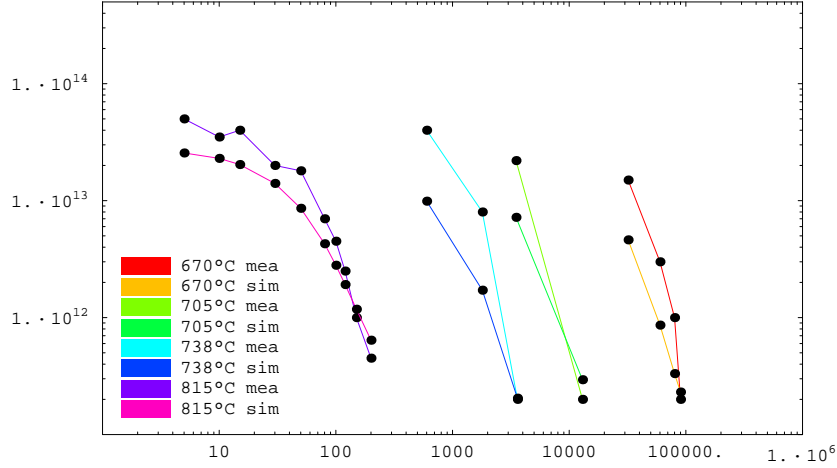


Fig. 3. Result for the low parameter set corresponding to parameter values shown in Table III. The logarithm (base 10) of the simulated and measured concentration [cm^{-3}] of interstitial clusters is shown depending on time [s].

two clusters and thus the expected values for the exponents are $\text{ifi} = 2 = \text{isfi}$. The second growth term $K_{\text{fc}}(I^{\text{ifc}}/I_{*}^{\text{isfc}})(C + \alpha I)^{\text{cf}}$ governs the case when an unclustered interstitials joins an interstitial cluster. Here we can expect the exponents to be unity. The second factor is a linear combination of C and I with an exponent.

Comparing (1) and (2), the growth term of (1), basically being a reaction constant times IC , is split into two parts providing greater flexibility: one depending on a modified interstitial supersaturation term and one depending on a modified interstitial supersaturation term times $(C + \alpha I)^{\text{cf}}$. In the dissolution term an exponent, which was later found to be 1, is added.

III. INVERSE MODELING AND RESULTS

Two points from the measurements in [3] were ignored since they were above the implanted dose. All measurements were viewed as one vector m . Let s be the vector of simulation results depending on the parameters p to be identified. The objective function $f(p)$ to be minimized was the quadratic mean of the element-wise relative error between a simulated point and a measured point, i.e.,

$$f(p) := \sqrt{\frac{1}{n} \sum_{k=1}^n \left(\frac{s_k(p) - m_k}{m_k} \right)^2}.$$

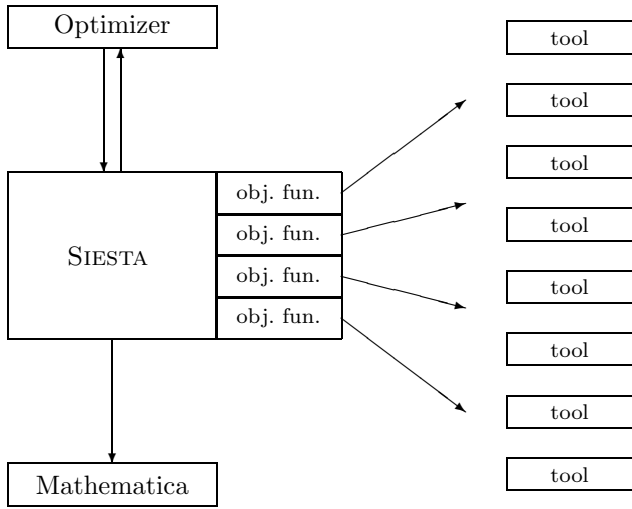


Fig. 4. Overview of SIESTA.

The variables of the objective function $f(p)$ are shown in Table II. The variables d_0 and dE determine the diffusivity $d_0 \cdot e^{-dE/kT}$ of interstitials in Silicon.

In order to reduce the time needed for the inverse modeling task, the optimization framework SIESTA was used. Its main tasks are optimizing a given objective function and parallelizing the executions of the objective function which usually entails calling simulation tools in a loosely connected cluster of workstations. SIESTA provides several local and global optimizers, the ability to define complicated objective functions, and finally an interface to MATHEMATICA for examining the results. Figure 4 shows an overview.

The optimization approach was to first identify reasonable ranges for the variables with great influence, namely energies and exponents. While identifying these ranges suitable starting points for gradient based optimization were found as well. Using these ranges and starting points the optimizations proceeded automatically including all variables.

It was soon found that changing cf and cr did not yield improvements and whenever these variables could be used by a gradient based optimizer, values very close to 1 resulted. The results described in Table III and Figure 2 were obtained for the high parameter set.

Similarly we carried out the same computations for the low parameter set, i.e., TSUPREM-4's default values. These results are shown in Table III and Figure 3.

IV. CONCLUSION

Starting with (2) and the measurements from [3] we adjusted a model for the formation and dissolution of Silicon self-interstitial clusters, namely

$$\frac{\partial C}{\partial t} = K_{fi} \frac{I^2}{I_*^2} + K_{fc} \frac{I}{I_*} (C + \alpha I) - K_r C,$$

with values from Table III. Although different values were also examined, the exponents in the first term were found to be equal to 2 ($ifi = 2 = isfi$), because two isolated interstitials can form a new cluster. Good results were achieved with $cf = 1$ and $ifc = 1 = isfc$, which means the rate of free interstitials joining already existing clusters depends linearly on the number of excess interstitials (interstitials above the equilibrium concentration) and a linear combination of the number of clusters and interstitials. Finally the exponent cr was found to be 1. This means that the rate of dissolution depends on the concentration of clustered interstitials and on the factor K_r .

The terms responsible for cluster formation in both models don't share a common structure, thus we finally compare the results for the dissolution term. In (1) the dissolution term is

$$-\frac{D_0 C}{a^2} e^{-(E_b + E_m)/kT},$$

where the values for E_b and E_m given in [1] are $E_b = 1.8\text{eV}$ and $E_m = 1.77\text{eV}$. $E_b + E_m = 3.57\text{eV}$ agrees very well with the values found for krE in Table III, namely 3.56997eV for the high parameter set and 3.84503eV for the low parameter set.

In order to give a summary, a refined model for the formation and dissolution of Silicon self-interstitial clusters was calibrated to published measurements for two different technologies (corresponding to two different sets of material parameters) and very good agreement was achieved.

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