6.7.58 Process Simulation - Atomistic

The diffusion of point defects, whose interactions can lead to the formation of extended defects, is a fundamental physical process at the root of most materials processing steps. Until recently, the diffusion process was modeled almost exclusively on the basis of the continuum approach and on partial differential equation (PDE) solvers. The main reason for taking such an approach was that it is less computationally expensive than any of its atomistic counterparts. However, the level of sophistication reached by today's materials processing technologies is calling for new modeling and simulation schemes, capable of handling the rich variety of interaction mechanisms that govern such complex processes at the atomic level. The Kinetic Monte Carlo technique seems particularly apt to fill in that gap.

1. The Kinetic Monte Carlo (KMC) Approach

Molecular dynamics (MD) is the most accurate atomistic simulation technique. However, due to the fact that it simulates all the lattice atoms and, most importantly, that it uses an almost constant timestep on the order of the femtosecond (10^{-15} s) , it cannot simulate the time scales involved in typical technological processing steps (seconds to hours). The kinetic Monte Carlo method, instead, is an event-driven technique, i.e., simulates events (e.g. diffusion hops) at random, with probabilities according to their respective event rates. In this way it self-adjusts the timestep as the simulation proceeds, just to be able to account for the fastest event present at that time. In what follows, the KMC simulator DADOS (Jaraiz *et al.* 1996, Jaraiz *et al.* 1998) will be used as a reference.

1.1 Simulation Scheme

Figure 1 illustrates the concept behind the KMC approach: the figure shows a high resolution TEM view (Eaglesham *et al.* 1994) of a silicon sample with a {311} extended defect embedded in the silicon atomic rows. In MD, all lattice and defect atoms are simulated. In KMC, only the atoms belonging to point or extended defects (represented as circles on the TEM view) are simulated. In the actual sample, all lattice atoms would be vibrating (with a period of about 10^{-13} s) and, from time to time (e.g. every 10^{-9} s), one of the isolated point defects would jump to a neighboring position where it might be captured by an adjacent extended defect. At even longer time intervals (e.g. every 10^{-3} s) a point defect would be emitted from the extended defect. To simulate this, KMC starts out with timesteps of about 10^{-9} s, since it only follows the defect atoms. In addition, the fast moving point defects disappear very quickly, leaving only the extended defect and allowing the timestep to automatically be raised to 10^{-3} s.

A key component in a KMC simulator is the event manager or "Scheduler", which is the procedure responsible for selecting the random events according to their event rates. Fig. 1 illustrates the selection procedure for a configuration consisting of 3 vacancies (V), 2 interstitials (I) and one {311} defect. Let's assume that the vacancy and interstitial jump rates are 1000 s⁻¹ and 100 s⁻¹ respectively, and the {311} emission rate is 10 s⁻¹. Then, to simulate 1 s we need to simulate a total of 3210 events. In addition, we have to pick a V with a probability proportional to 3000/3210, an I with a probability proportional to 200/3210.

A KMC simulator consists of a 3D simulation box, of dimensions ranging from tens of nanometers to a few microns, where point defects can be created and allowed to jump and interact. For instance, to simulate an ion implantation step, a BCA (Binary Collision Approximation) code can be used to generate the coordinates of the I's and V's for each cascade, allowing for some annealing between cascades to account for dose rate effects. Or I's can be generated at one of the box surfaces to simulate an oxidation step.

1.2 Defect Types

In DADOS, each defect atom is represented by a point, with coordinates (x, y, z) and a common interaction radius, in a 3D simulation box. It is, therefore, very easy to build any type of defect by either the transformation of existing point defects or by agglomerating jumping point defects to form an extended defect like the {311} shown in Fig. 1. Extended defects can be modeled replicating the actual geometry of the defect: vacancies can form spherical clusters (voids), interstitials can grow elongated stripes ({311}'s), or planar dislocation loops and stacking faults. Modeling the actual geometry improves the accuracy of the emission and capture rates, and can become essential in the proximity of the surface. A free surface is treated as a particular type of extended defect, and is included in the Scheduler with I and V emission rates

derived from the surface area and the formation energy of the corresponding point defect. The interaction or capture region of an extended defect is the superposition of the capture spheres of the constituent particles. Finally, each type of capture process can have an associated capture energy barrier.

1.3 Input Parameters

In the current version of DADOS, a unique capture radius is used for all particles, equal to the jump distance, λ , which is taken to be the second nearest neighbors distance in silicon (3.84 Å). As an example of event rate, the interstitial jump rate is given by

$$J_{rate,I} = 6 \times D_0 \times exp(-E_{mig,I}/kT) / \lambda^2$$

where D_0 is the diffusivity prefactor and $E_{mig,I}$ is the interstitial migration energy. Figure 2 represents the total energy of a system consisting of one boron and one silicon interstitial atom, as the system goes through different configurations. The intermediate configuration corresponds to an IB pair that is assumed to be immobile, whereas B_i stands for a mobile interstitial boron. The activation energy for the emission of a B_i from the IB pair is:

$E_{act,Bi} = E_{bind,Bi} + E_{mig,Bi}$

where $E_{bind,Bi}$ is the binding energy of the interstitial boron. These energies, obtained from ab initio calculations (Zhu *et al.* 1996) or estimated by fitting experimental data, are then used in the Scheduler to calculate the event rates and decide which event to perform next.

In addition to point defects, a full KMC simulator should implement models for a variety of extended defect types like the above mentioned surfaces, clusters and complexes (e.g. B_mI_n). Fig. 3 is a plot of the activation energy for the emission of an interstitial from interstitial clusters of different sizes, as derived from experimental measurements (Cowern *et al.* 1999a). The binding energy for a vacancy cluster (void) of size N is the energy difference between two configurations for N vacancies: a single vacancy plus a size N-1 void, and a size N void. Assuming that the void energy is proportional to the number of vacancies at its surface, taking 3.65 eV as the vacancy formation energy at the free surface and choosing the prefactor to fit the experimental activation energy for the divacancy, the vacancy binding energy is (Jaraiz *et al.* 1998)

$$E_{\text{bind},V} = 3.65 + 4.9 \times [(N-1)^{2/3} - N^{2/3}]$$

Although this equation was used for all void sizes, a KMC simulator can equally well use a table of discrete values, just like in the case shown in Fig. 3 for the interstitial cluster energies.

Finally, Table I collects some of the parameter values used in the current version of DADOS for the boroninterstitial complexes, $B_m I_n$ (Pelaz *et al.* 1997).

2 Simulation examples

The capabilities of the KMC approach as a materials process simulator, establishing a direct link between atomistic parameters and standard process experimental data, have been explored over the last few years with the most encouraging results. The following examples show some of the unique capabilities of this type of process simulator.

2.1 Voids

High dose implantation of heavy ions at elevated temperatures (to prevent amorphization) can lead to the agglomeration of vacancies to form large vacancy clusters (voids), with rounded shapes that are visible by TEM. Due to the momentum of the heavy ion, the silicon atoms are knocked deeper into the substrate leaving behind a vacancy rich region near the surface, where the voids are formed. Voids can be used as gettering centers because their internal surface behaves like a clean silicon surface. Figure 4 (Holland and White 1991) shows a cross-sectional view of a 100 keV, 10^{16} cm⁻² As⁺ implant. Beam heating with a high flux ion beam was used to prevent amorphization. A 45 nm region can be identified, extending from the surface, which contains a high density of voids followed by a band of dislocations extending up to about 200 nm. Although in this case the temperature can only be roughly estimated, the DADOS simulation,

shown at the same scale in the bottom figure, also predicts the formation of voids and interstitial clusters within the same depth ranges under those implant conditions.

2.2 {311} defects

Figure 5 (top) shows a plan view TEM of a 40 keV, 5×10^{13} Si⁺/cm² implant after annealing at 800 °C for 30 s (Stolk *et al.* 1995) and the corresponding DADOS simulation (bottom). This type of simulator has been shown to be able to yield very accurate quantitative predictions of the time evolution of the interstitial defects (Cowern *et al.* 1999b). In addition, and unlike the continuum models, this simulator also describes the actual geometry of the defects, which can play an important role in low energy implants, where their size is comparable to the distance to the surface.

2.3 The "+1" model

The damage generated during ion implantation induces transient enhanced diffusion (TED) of dopants that diffuse interstitially, like boron. In the current trend towards small thermal budgets, it has become essential to model TED in order to predict device profiles. In spite of the complexity of the process associated with the annealing of the damage, the "+1" model (Giles 1991) has been very successful for predicting TED. According to that model, only one excess interstitial is left per implanted ion, since the ion becomes substitutional and the Frenkel pairs quickly recombine during annealing. This empirical rule, also verified experimentally by counting the number of interstitials in {311} defects (Eaglesham *et al.*1994), was first corroborated theoretically by KMC simulations of a 40 keV, 5×10^{13} Si⁺/cm² room temperature implant followed by an 800 °C anneal (Jaraiz *et al.* 1996). There are conditions, however, where the "+n" factor is experimentally known to significantly deviate from the +1 rule. KMC simulations can, in those cases, help understand and quantitatively predict the effective "+n".

For instance, Figure 6 (Pelaz *et al.* 1999) is a plot of the total number of interstitial hops per lattice site versus the implanted dose, for a 10 keV Si implant, after a 10 min anneal at 800 °C. The number of interstitial hops per lattice site is proportional to the time averaged diffusivity of interstitial diffusing dopants like boron. In the figure, the "+n" factor is defined as the ratio between the number of hops using the total damage to that using only the "+1" model. For very low doses the effective +n increases as the overlap between cascades decreases and interstitials can hop longer distances before they recombine. In the low dose limit, the +n saturates at the value corresponding to isolated cascades interacting with the surface only.

As another example, Figure 7 (Pelaz *et al.* 1998), shows the enhanced boron diffusivity as measured in the experiment (Griffin *et al.* 1993) compared with the total number of silicon interstitial hops per lattice. Simulations including all the Frenkel pairs generated in the cascades and using only the +1 model, are plotted. Notice the deviation of the +1 model from the experimental values and the excellent prediction of the full KMC simulations.

In these simulations, the advantage of the KMC versus the continuum approach relies on the fact that the former is almost insensitive to the particular diffusivity values used. This is so because it mimics the random walk and, therefore, reduces the recombination problem to the probability that an interstitial meets a vacancy along its random path. Now, that probability is a function of the jump distance and of the capture radius, which should not be off by more than a factor of, say, two or three. The diffusivities and reaction rates used in the continuum approach, on the contrary, can be off by orders of magnitude.

2.4 Boron diffusion and clustering

A notable progress was also achieved in the long standing problem of boron diffusion and clustering through the use of KMC simulations (Pelaz *et al.* 1997). Besides TED, implanted boron also exhibits the problem of incomplete electrical activation, which was attributed to clustered boron although there was little understanding of the specific mechanisms leading to the coalescence of the electrically inactive component. In this case, the easiness provided by the KMC simulator for implementing and testing complex mechanisms was crucial to find a model whereby boron clustering is initiated by the nucleation of immobile cluster "precursors" consisting of a boron atom and several silicon interstitials, for example BI₂. Figure 8 (Pelaz *et al.* 1997) shows the SIMS profiles in a sequence of anneal times at 800 °C along with the simulation results. Notice the excellent agreement between the model and the experiment over the entire run. The predicted electrically inactive or clustered boron also agrees well with spreading resistance profilometry data (not plotted in the figure). This model provides parameters and suggests simplified mechanisms that can be implemented in continuum process simulators.

2.5 3D process simulation: 50 nm MOSFET

The complexity of the atomic level interaction mechanisms involved in today's semiconductor device processing is a subject of concern for the microelectronics industry, as already manifested in the 1997 SIA Roadmap (NTRS 1997 p. 188): "Continuum physics models are no longer sufficient below 100 nm. Tools are needed for the physical and chemical processes at an atomic level". Furthermore, the discreteness of the channel dopants has been shown to give rise to both a shift of the threshold voltage (as compared to the prediction from the continuum approach) and to an asymmetry in drain current upon interchanging the source and drain (Wong and Taur 1993). Figure 9 is a sketch of the simulated region of a 50 nm N-MOSFET including the 40-nm S/D extension and half the channel region. The processes simulated are (1) 5 keV, 10¹⁴ As/cm² S/D extension implant, (2) 70 keV, 10¹³ BF₂/cm² SPI implant and (3) 10s, 950 °C anneal. Figure 10 shows a snapshot of the simulation after 25 ms annealing, time at which the average {311} size reaches its maximum. This configuration is analyzed in four separate views. Figs. 10 (a) and (b) are plan views of the {311} defects and As implanted atoms, respectively. Figs. 10 (c) and (d) are cross sectional views. Assuming non-amorphizing conditions, microvoids form near the surface whereas interstitials are pushed beyond the As implant range due to the heavy As ion mass. The Si interstitials generated by the arsenic implant induce TED on the boron already present in the channel, depleting the channel to S/D transition region and leading to the reverse short channel effect, of detrimental consequences in deep sub-micron devices. The KMC simulation of sub-0.1 µm devices can be even more computationally efficient than the full model 3D continuum approach and, in addition, it provides a simulation with an unprecedented level of detail. In particular, the KMC method is especially apt for the study of atomic scale spatial correlation associated to the discreteness of the dopants. In summary, the KMC technique can also be used to implement a new type of device processing simulator, that looks particularly well suited to tackle the problems posed to today's TCAD systems.

> M. Jaraiz [E.T.S.I. Telecomunicacion, Univ. of Valladolid Valladolid, Spain]

3 Bibliography

Cowern N E B, Mannino G, Stolk P A, Roozemboom F, Huizing H G A, van Berkum J G M, Cristiano F, Claverie A, Jaraiz M 1999a Energetics of self-interstitial clusters in Si. *Phys. Rev. Lett.* **82**, 4460-3

Cowern N E B, Jaraiz M, Cristiano F, Claverie A, Mannino G 1999b Fundamental diffusion issues for deep-submicron device processing. *Int. Electron Dev. Meeting Proc.*-99, 333-6

Eaglesham D J, Stolk P A, Gossmann H J, Poate J M 1994 Implantation and transient B diffusion in Si: The source of the interstitials. *Appl. Phys. Lett.* **65**, 2305-7

Giles M D 1991 Transient phosphorus diffusion below the amorphization threshold. *J. Electrochem. Soc.* **138**, 1160-5

Griffin P B, Lever R F, Huang R Y S, Kennel H W, Packan P A, Plummer J D 1993 Species, dose and energy dependence of implant induced transient enhanced diffusion. *Int. Electron Dev. Meeting Proc.*-93, 295-8

Holland O W, White C W 1991 Ion-induced damage and amorphization in Si. *Nucl. Instr. and Meth. B* **59/60**, 353-62

Jaraiz M, Gilmer G H, Poate J M, de la Rubia T D 1996 Atomistic calculations of ion implantation in Si: Point defect and transient enhanced diffusion phenomena. *Appl. Phys. Lett.* **68**, 409-11

Jaraiz M, Pelaz L, Rubio E, Barbolla J, Gilmer G H, Eaglesham D J, Gossmann H J, Poate J M 1998 Atomistic modeling of point and extended defects in crystalline materials. In: Cowern N E B, Jacobson D C, Griffin P B, Packan P A, Webb R P (eds.) *Mater. Res. Soc. Symp. Proc.* Materials Research Society, Warrendale, Pennsylvania, pp. 43-53

National Technology Roadmap for Semiconductors (NTRS) 1997. Semiconductor Industry Association.

Pelaz L, Jaraiz M, Gilmer G H, Gossmann H J, Rafferty C S, Eaglesham D J, Poate J M 1997 B diffusion and clustering in ion implanted Si: The role of B cluster precursors. *Appl. Phys. Lett.* **70**, 2285-7

Pelaz L, Gilmer G H, Jaraiz M, Herner S B, Gossmann H J, Eaglesham D J, Hobler G, Rafferty C S, Barbolla J 1998 Modeling of the ion mass effect on transient enhanced diffusion: Deviation from the "+1" model. *Appl. Phys. Lett.* **73**, 1421-3

Pelaz L, Gilmer G H, Venezia V C, Gossmann H J, Jaraiz M, Barbolla J 1999 Modeling of the effects of dose, dose rate, and implant temperature on transient enhanced diffusion. *Appl. Phys. Lett.* **74**, 2017-9

Stolk P A, Gossmann H J, Eaglesham D J, Poate J M 1995 Implantation and transient boron diffusion: The role of the silicon self-interstitial. *Nucl. Instr. and Meth. B* **96**, 187-95

Wong H S, Taur Y 1993 Three-dimensional "atomistic" simulation of discrete random dopant distribution effects in sub-0.1um MOSFET's. *Int. Electron Dev. Meeting Proc.*-93, 705-8.

Zhu J, de la Rubia T D, Yang L H, Mailhiot C, Gilmer G H 1996 Ab initio pseudopotential calculations of B diffusion and pairing in Si. *Phys. Rev. B* **54**, 4741-47

Table 1.

Simulation parameters for B-I agglomerates. $E_{n,m}$ is the potential energy of a $B_n I_m$ complex. Energies are in eV.

$D_{Bi} = 10^{-3} \exp(-0.5)$	$(3/kT) \text{ cm}^2/\text{s}$	Ebinding(1	BI)=1,	Ebinding(E	BI ₂)=1.2	
$E_{2,0}=0.0$	E _{2,1} =-2.1, E _{barrie}	er=0.5	$E_{2,2}=-4.8$	8		
$E_{3,0}$ =-0.8	$E_{3,1}$ =-4.0		$E_{3,2}=-5.5$	5,	E _{3,3} =-6.8	
E _{4,0} =-1.2	$E_{4,1}$ =-5.0		E _{4,2} =-6.4	4,	E _{4,3} =-7.4,	E _{4,4} =-8.5

 $E_{n,m}$ =-0.2n-2.0m, n≥5; $E_{barrier}$ =1, n=5

Figure captions

Figure 1.

TEM view of an extended {311} defect in silicon (Eaglesham *et al.* 1994). Circles represent the (defect) atoms simulated by the KMC method. As an example, the figure illustrates the emission of an interstitial (I) from the {311} defect and its eventual recombination with one of the vacancies (V) present in the sample.

Figure 2.

Total energy of a boron atom and a silicon interstitial as the system goes through different configurations. A (mobile) interstitial point defect, jumping with a migration energy $E_{mig,I}$, can find a substitutional B atom and give rise to an immobile IB pair. Subsequently, the IB pair can transform into an interstitial boron atom, migrating with an energy $E_{mig,Bi}$. $E_{b,Bi}$ and $E_{act,Bi}$ are the binding energy of the Bi defect and the activation energy of the IB \rightarrow Bi process, respectively.

Figure 3.

Emission energies of interstitial clusters as a function of the size, as derived from experimental measurements at three different temperatures (Cowern *et al.* 1999a).

Figure 4.

Cross-sectional TEM of a beam-heated, 100 keV, 10^{16} cm⁻² As⁺ implant (Holland and White 1991), compared with the corresponding simulation using DADOS, drawn to the same scale (units are nm).

Figure 5.

Plan view TEM micrograph (Stolk *et al.* 1995) (a) and DADOS simulation (b) of a 40 keV 5×10^{13} cm⁻² silicon implant after a 30 s annealing at 800 °C, exhibiting {311} defects.

Figure 6.

Total number of interstitial hops per lattice site versus the implanted dose, for a 10 keV Si implant, after a 10 min anneal at 800 °C. The results of a full Monte Carlo simulation are compared with those of a simulation using the "+1" approximation. The "plus factor" is given by the ratio of the two curves (Pelaz *et al.* 1999).

Figure 7.

Experimental time averaged diffusivity (Griffin *et al.* 1993) and simulated total number of interstitial hops per lattice site for (a) equal range implants (R ~ 45 nm: 15 keV B, 35 keV P, 80 keV As) and (b) equal energy implants (35 keV), after 120 min at 750 °C anneal curves (Pelaz *et al.* 1998).

Figure 8.

Experimental SIMS profiles (thin lines) and DADOS simulation profiles (thick lines) for a boron doped layer after a 40 keV 9×10^{13} cm⁻² silicon implant and anneal at 800 °C. Thick dashed lines are the simulated boron in clusters (Pelaz *et al.* 1997).

Figure 9.

50 nm N-MOSFET corresponding to the process described in the text. The simulated region is also indicated in the figure.

Figure 10.

Simulated atomistic configurations of the device of Figure 9, after a short annealing of 25 ms. (a) and (b) are plan views of the {311} defects and As implanted atoms, respectively, while (c) and (d) are their respective cross sectional views.