Kinetic Monte Carlo Simulations for Defects Diffusion in Ion-implanted Crystalline

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Abstract

An atomistic process modeling, Kinetic Monte Carlo simulation, has the advantage of being both conceptually simple and extremely powerful. Instead of diffusion equations, it is based on the definitions of the interactions between individual atoms and defects. Those interactions can be derived either directly from molecular dynamics, first principles calculations, or from experiment.

In this paper, as a simple illustration of the kinetic Monte Carlo we simulate defects (self-interstitials and vacancies) diffusion after ion implantation in Si crystalline.

Ⅰ. Introduction

The level of semi-conductor devices reached by recent materials processing technology calls for new modeling and simulation schemes capable of handling the variety of atomic interactions because classical process simulations can not simulate accurately nano-scale processing. So, new modeling and simulation tools are needed for the accurate nano-scale process simulations at an atomic level. We describe the kinetic Monte Carlo (KMC) technique for the diffusion of point defects (self-interstitials, vacancies). KMC has been proved to be extremely powerful as a direct bridge between first principles calculations (Ab-initio methods) and experimental data.

Ⅱ. Kinetic Monte Carlo approach and input data

After ion implantation, various defects are generated in silicon crystalline. So, annealing has to be taken for the electrical activation of damaged lattice atoms in Si and dopants (B, As, F). In fabrication, to predict an accurate performance of new devices, many simulation techniques have been used. Usually ab-initio calculations or classical MD (molecular dynamics) simulation techniques are the most accurate. However, due to the fact that it simulates all the lattice atoms and that it uses an almost constant time step on the order of femto-second (10^{-15} sec). It can not simulate the time scales involved in typical technological processing (second to hours). The kinetic Monte Carlo method, on the contrary, is an event-driven technique, i.e., simulate events at random with probabilities according to the corresponding event rates. In this way it self-adjusts the reasonable time step as the simulation proceeds

Ⅲ. Simulation scheme

An atomistic diffusion simulator basically consists of a simulation box, of dimensions ranging from tens of nano meters to a few microns (23.5 in this work), containing a variety of point defects (self-interstitials, vacancies) and extended defects. To the contrary of MD, in this kinetic Monte Carlo scheme lattice atoms are regarded as a background and are not included in the simulation.

In this implementation, we consider the only point defects (self-interstitials, vacancies) in ion-implanted Si. One of the isolated point defects would jump to a neighboring site and can be captured by the extended defect or recombined by the opposite type of defect (I, V). Since KMC method only simulates the defects. It starts out with time steps on the order of femto second. In addition, the fast moving point defects disappear very quickly, leaving only the extended defects.

The only event that a point defect (I, V) can perform is a jump. Their jump rate is given by

$$J_{rate} = 6 * D_0 * \exp(-E_m / KT) / \lambda^2$$

Here D_0 is the diffusivity pre-factor, E_{mig} is the event migration energy and λ the jump distance (2.35Å).

In our defect diffusion simulation, there are only two types of defects, self-interstitials and vacancies. Diffusivities and energy barriers are given by

$$D_i = 1.717 \text{ 1/fs}$$

$$E_i = 1.37 \text{ eV}$$

$$D_v = 0.001282 \text{ 1/fs}$$

$$E_v = 0.1 \text{ eV}.$$

These parameters are changed by temperature and proper at 1000K.

We consider the activated processes discussed above. If the probability of next jump to occur is independent of the previous history, and the same at all times, the transition probability is a constant. Then the process is a so-called Poisson process. To derive the time dependence, consider a single object with a uniform transition probability r. Let f the transition probability density, which gives the probability rate at which the transition occurs at time t. The change of f(t) over some short time interval dt is proportional to r, dt and f because f gives the probability density that the object still remains at time t.

$$df(t) = -rf(t)dt$$

and the solution is given by with boundary conditions

$$f(t) = re^{-rt}, f(0) = r$$

Therefore, we update the simulation time with (t = t + Δt) according to event hopping rate:

$$\Delta t = -\frac{\log u}{R}$$

Here, u is a random number. We select an event according to the event hopping rate and KMC is proper to simulate non-uniform time evolution processes.

Ⅳ. Simulation results

After ion implantation at 2 x 10^4 ions/cm^2 dose rate (Fig. 2), the defects hopping distance is 2.35 (it assumes that defects are transited only in 6 directions) and the length for the recombination is 4 . After 10^9 fs, many defects are recombined and vanish. And the rate of recombination is dependent on annealing temperature (Fig. 1) i.e. in high temperature (2000K), defects (self-interstitials and vacancies) are recombined rapidly.

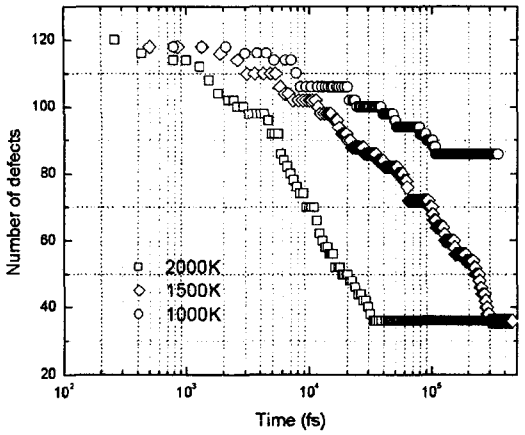

Fig 1. Plot showing the number of defects dependent on temperature.

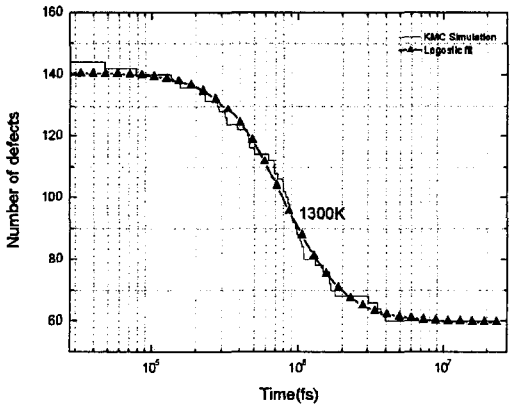

Fig. 2 Plot showing the number of defects

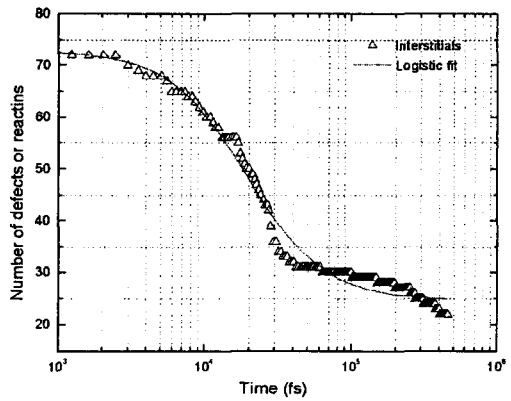

Fig. 3 Plot showing the number of self-interstitials according to time increment.

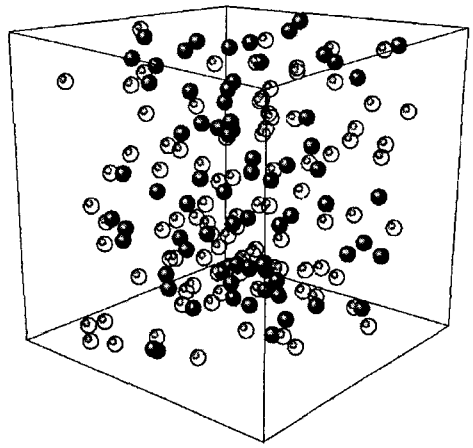

Fig. 4 Plot showing the 3D snap-shot of the defect distribution, just before annealing process: 2 x 10^4 ions/cm^2 Ion implantation. White circles represent vacancies and dark greys interstitials.

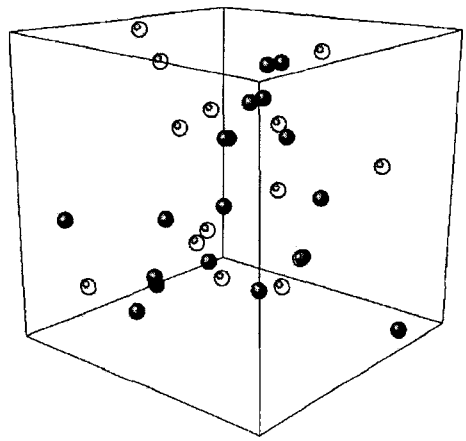

Fig. 5 Plot showing the snap-shot of the defects distribution which are declined by recombination (I, V) after 10^9 fs.

In this work, the only basic defects (self-interstitials and vacancies) are considered. To estimate more accurate and reasonable results, we should add more defect models (clusters, {311} defects, dislocation loop). These models are being added now to our code.

V. Conclusions

Until recently, diffusion simulators have been only based on continuum models and partial differential equations solvers.

However, Kinetic Monte Carlo methods, applied to materials processing simulations, allow the direct use of parameters obtained from first principles calculations or experimental data, thus establishing a bridge that can be highly beneficial for both the computational materials science and the microelectronics industry communities. KMC can nowadays provide an effective way to simulate microelectronics processing measurements.

VI. References

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