

Acceleration of Lattice Monte Carlo Simulations and Application to Diffusion/Clustering of As at High Concentrations

Scott T. Dunham and Zudian Qin

Department of Electrical Engineering, University of Washington
Seattle, WA 98195
dunham@ee.washington.edu

Abstract

Kinetic lattice Monte Carlo (KLMC) simulations enable practical atomic-scale modeling of device fabrication processes. In this paper, we discuss implementation of an acceleration algorithm which can provide orders of magnitude speed-up. We apply the result to diffusion and clustering of As at very high doping levels, which are critically important in the formation of ultrashallow junctions.

1. Introduction

Kinetic lattice Monte Carlo (KLMC) simulations are a promising approach for atomic-scale modeling of device fabrication processes [1–4]. By considering only the transitions (and not lattice vibrations) associated with the defects and impurities present in the system, KLMC is able to overcome the time-scale limits associated with molecular dynamics to consider macroscopic systems and time scales. In previous work, we have demonstrated the ability to model the fabrication of deep submicron device structures [2]. However, KLMC simulations are still much more CPU intensive than continuum simulations. In this paper, we discuss implementation of an acceleration algorithm, and we apply the result to a problem which has led to controversy in the literature [1, 5] and is critical for formation of low resistance shallow junctions: diffusion and clustering of As at very high doping levels.

The KLMC system considers impurities and point defects located at silicon lattice sites. The energy of the system is defined based on the atomic scale arrangement, with parameters determined from *ab-initio* calculations and/or experimental observations. The system evolves through transitions from one atomic configuration to the next. The rates of these transitions can be determined based on the migration barriers and changes in system energy associated with the transition: $\nu = \nu_0 \exp(-E_m/kT) \exp[(E_i - E_f)/2kT]$, where E_m is the migration energy, E_i is the energy of the initial configuration and E_f is the configuration of the final state. At each time step, a transition is chosen from the full possible set based on the relative rates, and the time step is advanced by the inverse of the sum of the rates [1, 4].

2. Acceleration Algorithm

For heavily As-doped material, the simulation spends the bulk of its time transitioning among a set of coupled low energy states associated with As_nV

complexes, without resulting in long-range diffusion or advancing the system rapidly forward in time (Fig. 1). To overcome this bottleneck, we can generalize the concept of a state to include a group of states which approaches local equilibrium via extensive sampling within the expected time for a transition out of the set [4]. In this case, we can immediately jump to transitions out of this group of states, with a correspondingly large time acceleration. More formally, a set of configurations \mathcal{K} can be replaced by a single effective state provided the transitions between members of the set are fast compared to transitions between a member of the set and configurations that are not members. In this case, the transition rate to a configuration j outside \mathcal{K} is

$$\nu(\mathcal{K} \rightarrow j) = \sum_{k \in \mathcal{K}} p_k \nu(k \rightarrow j) = \sum_{k \in \mathcal{K}} \exp(-[E_k - E_{\mathcal{K}}]/kT) \nu(k \rightarrow j), \quad (1)$$

where p_k is the probability of configuration k within set \mathcal{K} , and $E_{\mathcal{K}} = -kT \ln[\sum_{k \in \mathcal{K}} \exp(-E_k/kT)]$. From a practical perspective, we check for existence of a group of tightly coupled states when the system revisits a given state with high frequency over a short time period. Starting from this state, the set of coupled states is then expanded automatically via the requirement that the rates out of the set are at least M times slower than rates within the set (typically, $M \sim 100$).

3. Simulation Results

We have applied this approach to simulation of diffusion of As at high concentrations. In our previous work based on As/V attraction at 1NN to 3NN separation [1], we found a rapid increase in diffusivity (beyond Fermi level effects) as the doping concentration increased above 10^{20}cm^{-3} which was in agreement with experimental results of Larsen *et al.* [6] (Fig. 2). However, List *et al.* [5] tried to reproduce these results and reported that the apparent As diffusivity actually dropped with doping concentration. They were only able to obtain enhancement as observed by Larsen *et al.* by eliminating 1NN binding, in contradiction to experimental [7] and theoretical [8] results. The reason for this discrepancy lies in the methods and time scales considered. In our previous work [1], we considered only very short time scales, before significant As/V cluster formation could occur. For longer times in a system with fixed V concentration (as analyzed by List *et al.*), the diffusivity drops sharply with doping due to formation of relatively immobile As_nV [3].

Because the period before clustering begins becomes extremely short as doping level rises, it is very difficult to get accurate statistics using this approach. We find that it is possible to consider more reasonable time scales and yet correctly extract the arsenic diffusivity versus concentration by recognizing that as clustering occurs, the equilibrium number of vacancies rises dramatically as well. We correct for this factor by scaling the time by the ratio of equilibrium to actual number of free vacancies in the system (Fig. 3). There is still a problem at high doping concentrations as vacancies get trapped in As_nV complexes. However, via use of the algorithm described above, we are able to accelerate

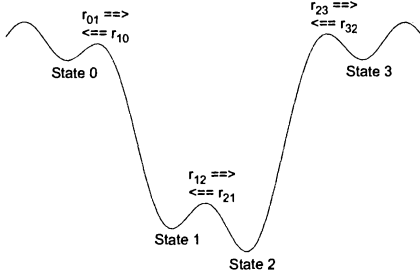


Fig. 1: Schematic of energy versus configuration for system with fast transitions between a small subset of states. If $r_{10}, r_{23} \ll r_{12}, r_{21}$, then a large number of steps will simply involve exchange between states 1 and 2. By detecting that a local equilibrium exists between these two states, we can ignore the r_{12}, r_{21} transitions and consider only the transitions out of the set (e.g., $r_{\kappa 0} = p_1 r_{10} = r_{21} r_{10} / (r_{21} + r_{12})$).

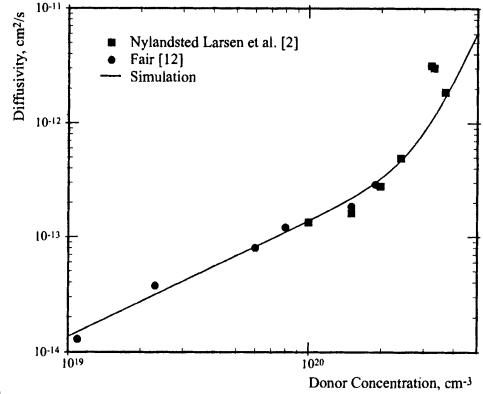


Fig. 2: Comparison of experimental measurement [6, 9] of arsenic diffusivity at 1050°C versus doping level to lattice Monte-Carlo simulations using short simulation times to avoid clustering [1]. The diffusivity for moderate doping levels is fit assuming diffusion via negatively-charged vacancies and then extrapolated to higher doping levels using the simulation results.

out of these states and thus simulate the long time periods needed to accurately extract equilibrium diffusivities.

For our simulations, we use arsenic/vacancy interactions out to 3NN from *ab-initio* calculations [8]. The results for normalized diffusivity versus arsenic concentration at 1000°C are shown in Fig. 4. We find a rapid increase in diffusivity above $2 \times 10^{20} \text{cm}^{-3}$, as in previous work [1] and experiments [6].

The acceleration algorithm enables practical simulation of large systems with strong binding energies. We use KLMC to analyze diffusion and clustering during annealing of laser or RTA activated junctions. In these systems, rapid arsenic deactivation is observed [10] due to As_nV cluster formation driven by the greatly enhanced diffusion at high concentrations described above. This process also requires vacancy generation as diffusion from the surface is much too slow to account for deactivation kinetics at short times and low temperatures. We also used KLMC simulations to explore the formation of As clusters which are favorable for enhanced Frenkel pair generation via kick-out of central silicon atom. We find that these structures arise naturally via interstitial-mediated diffusion of As which is enhanced by the same Si kick-out process. By including I kick-out, we are able to use KLMC for atomistic modeling of diffusion and clustering of As at high concentrations.

References

- [1] S. T. Dunham and C. D. Wu, J. Appl. Phys. **78**, 2362 (1995).

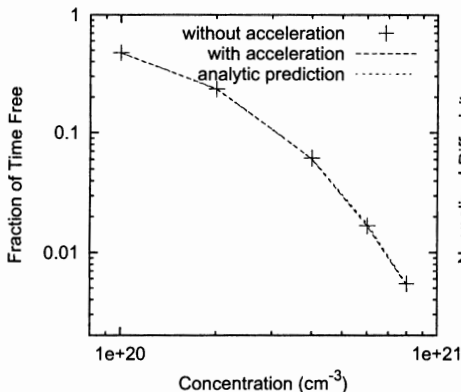


Fig. 3: Comparison of fraction of time that a vacancy is free from interactions with arsenic atoms as function of doping concentration calculated via three different methods: standard simulation without acceleration, simulation with acceleration, and analytic expression based on system probabilities. In all three cases, the results are indistinguishable, demonstrating the accuracy of both the acceleration algorithm and the analytic prediction.

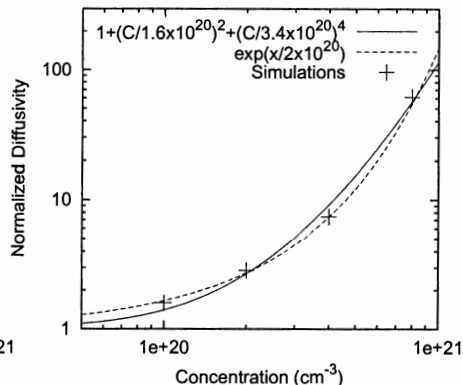


Fig. 4: Simulated diffusivity of As versus doping concentration normalized by dividing by normal Fermi-level dependent diffusivity ($\propto n/n_i$). The results are based on *ab-initio* As/V binding energies at $T = 1000^\circ\text{C}$. A rapid increase of diffusivity with polynomial or exponential doping dependence is seen.

- [2] M. M. Bunea and S. T. Dunham, in **Semiconductor Process and Device Performance Modeling**, S. Dunham and J. Nelson, eds. (Mat. Res. Soc. Proc. **490**, Pittsburgh, PA, 1998) pp. 3–8.
- [3] M. M. Bunea and S. T. Dunham, in **Defects and Diffusion in Silicon Processing**, S. Coffa, T. Diaz de la Rubia, C. Rafferty, and P. Stolk, eds. (Mat. Res. Soc. Proc. **469**, Pittsburgh, PA, 1997) pp. 353–358.
- [4] A. Horsfield, S. T. Dunham and H. Fujitani, in **Multiscale Modeling of Materials**, V. Bulatov, T. de la Rubia, N. Ghoniem, E. Kaxiras and R. Phillips, eds. (Mat. Res. Soc. Proc. **538**, Pittsburgh, PA, 1999).
- [5] S. List and H. Ryssel, *J. Appl. Phys.* **83**, 7585 (1998).
- [6] A. Nylandsted Larsen, K. Kylesbech Larsen, P. E. Andersen, B. G. Svensson, *J. Appl. Phys.* **73**, 691 (1993).
- [7] M. Hirata, M. Hirata and H. Saito, *J. Phys. Soc. Jap.* **27**, 405 (1969).
- [8] O. Pankratov, H. Huang, T. D. de la Rubia and C. Mailhot, *Phys. Rev. B*, **56**, 13172 (1997); J. S. Nelson, P. A. Schultz and A. F. Wright, *Appl. Phys. Lett.* **73**, 247 (1998); M. Berding, A. Sher, *Phys. Rev. B*, **58**, 3853 (1998); J. Xie and S.P. Chen, *J. Appl. Phys.* **87**, 4160 (2000).
- [9] R. B. Fair in **Impurity Doping Processes in Silicon**, ed. F. F. Y. Yang (North-Holland, New York, 1981) p. 315.
- [10] Scott Luning, PhD thesis, Stanford University (1996).