Linking of Atomistic Modeling to Macroscopic Behavior for Front End Processes

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ABSTRACT

In this work, we review efforts to make effective use of atomistic calculations for the advancement of VLSI process simulation. We focus on front-end processes such as defect mediated dopant diffusion which play a large role in determining device behavior.

Keywords: diffusion, point defects, lattice Monte Carlo, transient enhanced diffusion, extended defects

INTRODUCTION

Accurately predicting submicron device structures resulting from advanced integrated circuit fabrication processes is a very challenging problem due to the large number of strongly interacting reactions, the dominance of non-equilibrium behavior, and the fine tolerances required. Great advances have been made in understanding ion implantation, defect-mediated dopant diffusion, extended defect kinetics and film growth along with their interactions, but many mysteries still remain. Atomistic techniques provide a range of powerful tools including *ab-initio* calculations based on density functional theory (DFT), ab-initio or semi-empirical tight binding (TB) calculations, empirical-potential molecular dynamics (MD), and kinetic Monte Carlo (MC). These tools have the potential to significantly advance the predictive capability of process simulators. However, substantial challenges must be overcome to make effective use of such calculations due to the wide gap which is present in the spatial and temporal scales. In this paper, we will discuss a range of methods for applying atomistic simulations to modeling of front end processes, with specific examples provided as illustrations.

DIRECT APPLICATION OF ATOMISTIC CALCULATIONS

We will start by discussing how the results of *ab-initio* or TB calculations can be used directly as a source of parameters for continuum simulations. To begin, it should be noted that the accuracy of these calculations is generally insufficient for their direct use in quantitative prediction of device structures as, for example, a ± 0.1eV uncertainty in activation energy leads to a range of nearly an order of magnitude in predicted parameter values at 800°C. Instead, their main role lies in identifying the most likely reaction paths and dominant or rate-limiting process among the complex array of possibilities.

The most direct example of using parameters from atomistic calculations is in estimating the properties of native point defects, interstitials and vacancies. While, the $D_\mathrm{I}C_\mathrm{I}^*$ or $D_\mathrm{V}C_\mathrm{V}^*$ products are well-established based on experimental observations, there have been dramatic discrepancies in the reported values of the diffusivities and equilibrium concentrations. Fundamental calculations have confirmed that interstitials diffuse rapidly, but also contradicted accepted thinking by concluding that vacancies diffuse even faster.

The fast diffusion of vacancies plays a critical role in the initial stages of ion implant annealing. As a result of the collision cascade, implant damage consists of nearly equal numbers of interstitials and vacancies at concentrations much higher ($\sim$100–1000 times) than that of the primary implanted species. During the initial stages of the anneal, most of the faster diffusing vacancies will recombine with interstitials. However, particularly for lower doses, some of the vacancies may find their way to the surface and recombine there. The result is that instead of just a +1 net interstitial excess due to the implanted ions, there remain an additional net interstitial excess equal to the number of vacancies which reached the surface. This leads to an initial effective $+N$ damage (where $N > 1$) and corresponding greater TED. As shown in Fig. 1, including this effect leads to the prediction of the dose dependence of TED [1], which is otherwise underestimated at low doses.

Another example of direct application of atomistic calculations to continuum simulations is boron interstitial cluster (BIC) formation. It is logical to expect boron to aggregate in association with interstitials due to size differences, but there exists an immense range of possible cluster structures, compositions and formation paths (and associated large number of potential model parameters). Zhu *et al.* [3] calculated BIC formation energies via *ab-initio* methods. By using those results to calculate which species are present in significant numbers under TED conditions, and how rapidly cluster concentrations can be expected to equilibrate with the point

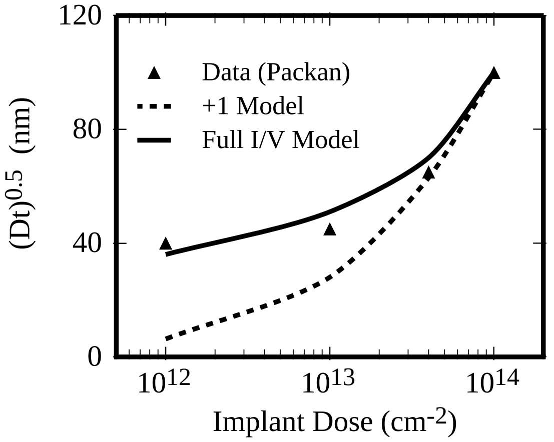

Figure 1: Dose dependence of TED measured for boron marker layers following 200 keV Si implants from Packan [2] compared to model simulations [1] which use a +1 or $+N$ initial net interstitial distribution, with the value of N obtained by considering the total initial defect concentrations and fast vacancy diffusion.

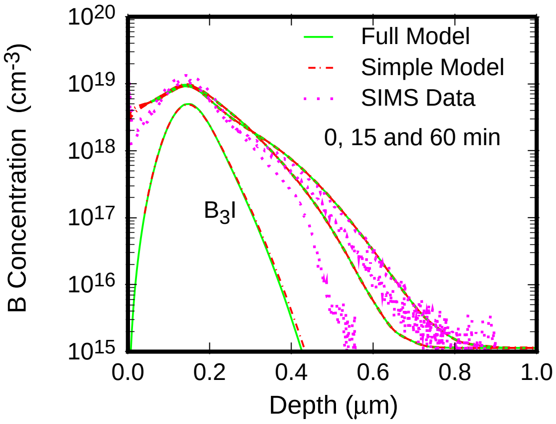

Figure 2: Comparison of full model [5] with the simplified model [4] for a 40keV $2 \times 10^{14} cm^{-2}$ B implant annealed at 800°C for 15 and 69 min. Also shown for comparison are SIMS data from Intel [7]. Note that the full model and simple model show indistinguishable final profiles. The BIC (B_3I) concentrations for the two models (shown after 1 h anneal) are also nearly identical.

defect concentrations, it is possible to derive a very simple BIC model [4]. The resulting system solves for the concentrations of only two immobile clusters (BI_2 and B_3I) and has only 3 parameters as compared to the full system with 8–10 equations and about 20 parameters (as in the work of Lilak *et al.* [5] and Pelaz *et al.* [6]), yet is able to fully duplicate the results of the full model (Fig. 2).

Ab-initio calculations are limited to relatively small systems and thus are unsuitable for application to larger extended defects such as {311} defects or dislocation loops (except for very high symmetry structures such as infinitely long {311} defects). To attack these problems, it is possible to use empirical or semi-empirical (e.g., TB) potentials [8]. Such calculations provide the dependence of energy on size which critically determines the time evolution of the extended defect size distribution. An example of such results obtained using the Stillinger-Weber potential are shown in Fig. 3 [9]. We can use this information in continuum simulations which otherwise have a parameter space equal to the number of defect sizes considered.

LATTICE MONTE CARLO

Although atomistic calculations can in many cases be used effectively in continuum simulations, many other processes occurring on the atomic scale are not accurately replicated in continuum models. At the same time, MD simulations are generally limited to times on the order of ns. To bridge this gap, we have developed a lattice Monte-Carlo (LMC) approach [10]–[14]. The strength of LMC is that at the fundamental level, most processes involve jumps between locally stable configurations. Thus, the underlying time scale is the hop frequency ($\sim 10^{-9}$s) rather than the vibration frequency ($\sim 10^{-13}$s). In addition, by considering only the behavior of mobile species (e.g., point defects), the number of active sites is many orders of magnitude smaller than the lattice density. Therefore, it is possible to maintain the underlying atomic structure and mechanisms and yet also consider system sizes and process times appropriate to submicron device fabrication. The parameters required for LMC are exactly the information available from *ab-initio* or MD calculations — interaction energies versus distance and transition rates as a function of configuration. LMC thus provides a natural bridge between fundamental calculations and macroscopic behavior for continuum simulations.

There are a number of processes for which such an intermediate level is necessary. For example, the reaction/diffusion equations used in continuum simulations assume a simplified picture of dopant/defect interactions. The widely-used pair diffusion (or fully-coupled) model assumes that dopants form pairs with point defects and then move as a unit, giving a dopant flux which depends on both the dopant and point defect gradient.

$$J_A^V = -D_{AV} K_{A/V} (C_V \nabla C_A + \gamma C_A \nabla C_V), \quad \gamma = 1 \quad (1)$$

However, vacancy-mediated diffusion is more complex than this since vacancies and dopants move in opposite directions during an exchange and need to separate to at least third-nearest-neighbor (3NN) distance to move again in a new direction. Through LMC simulations of dopant migration in a vacancy gradient, we find that

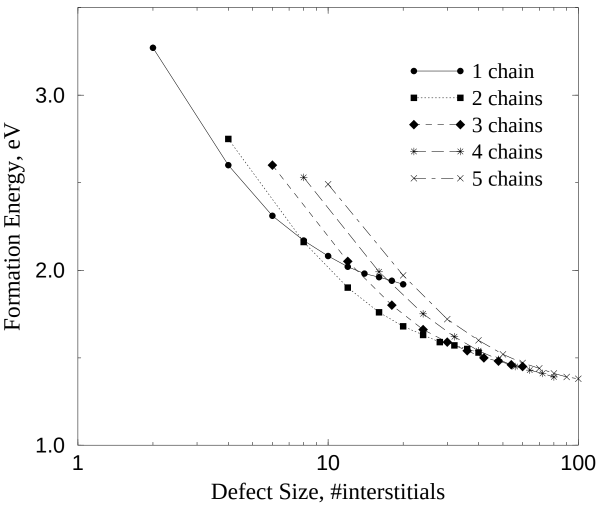

Figure 3: Formation energy per interstitial for $\{311\}$ for different defect widths (number of parallel $\langle 110 \rangle$ interstitial chains) with respect to the number of interstitials incorporated [9]. The optimum defect width increases with defect size. However, there is only small gain in energy for widening more than up to width 3 or 4.

Eq. 1 is valid for phosphorus, but that $\gamma < 1$ for arsenic (particularly at higher T) [11], [12]. The reason for this difference can be attributed to differences in the dopant/vacancy interactions as obtained from *ab-initio* calculations [15] (Fig. 4). For arsenic, the first dopant/vacancy exchange is likely to move the dopant *up* the vacancy gradient. Subsequent hops move the dopant *down* the pair, and thus vacancy, gradient. The first hop reduces γ, especially if the pair only makes a few hops before dissociating (as at higher T). For phosphorus, the large exchange barrier removes the first-hop bias, giving $\gamma = 1$.

Another area in which LMC is useful is for considering collective effects, such as the enhanced diffusion due to interactions of defects with multiple dopants in heavily doped material. We have found that LMC simulations of vacancy-mediated dopant diffusion using dopant/vacancy interactions as in Fig. 4 lead to greatly enhanced diffusion for very high doping levels ($> 2 \times 10^{20}\mathrm{cm}^{-3}$) [10]. These results are in agreement with the observations of Larsen *et al.* [16] of enhanced diffusion of As, Sb, Sn and Ge in heavily P-doped material (Fig. 5).

LMC simulations enable the consideration of the discrete nature of point and extended defect distributions. Following ion implantation, the initial locations of interstitials and vacancies resulting from the collision cascade are strongly correlated, especially for low doses. These correlations affect the numbers of defects which remain following initial Frenkel pair recombination as

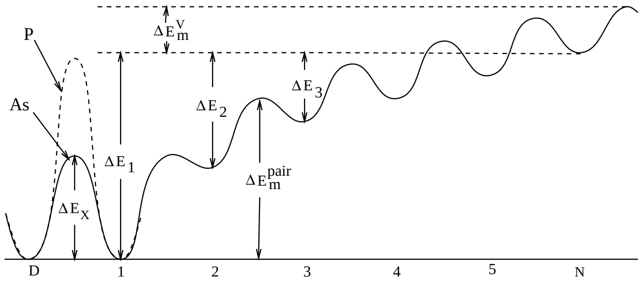

Figure 4: Schematic illustration of energy versus separation for dopant/vacancy complexes based on *ab-initio* calculations [15]. The dopant/vacancy pair must separate to 3NN distance for long-range migration. For arsenic, the migration barrier for the complex is associated with the 2NN/3NN transition. However, for phosphorus the large dopant/vacancy exchange barrier makes that process the rate-limiting step.

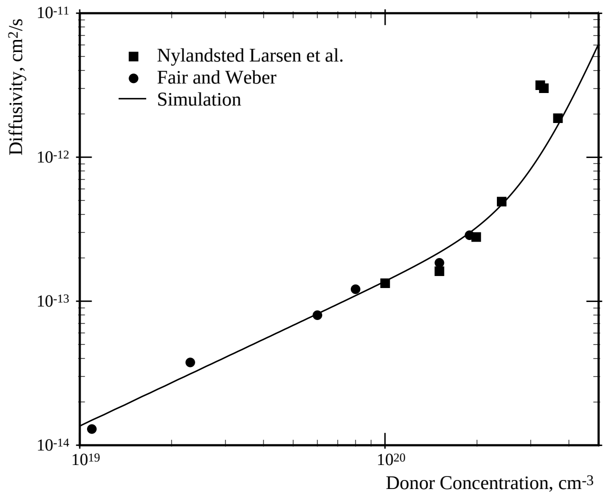

Figure 5: Comparison of LMC predictions to experimental measurement of arsenic diffusivity at 1050°C versus doping level [16], [17]. The diffusivity for moderate doping levels is fit assuming diffusion via negatively-charged vacancies and then extrapolated to higher doping levels using the LMC simulation results.

illustrated in Fig. 6 [14].

Reduced device dimensions and thermal budgets greatly reduce computation times for LMC simulations, while requiring the inclusion of complex non-equilibrium behavior that makes continuum simulations more computationally expensive. Thus LMC simulations become a realistic alternative for simulation of deep submicron structures. 3D LMC simulations of sub-100nm nMOS structures have already been demonstrated [13]. Such atomistic simulations will become necessary for deep submicron devices because the modest number of dopants and defects present lead to significant variations in de-

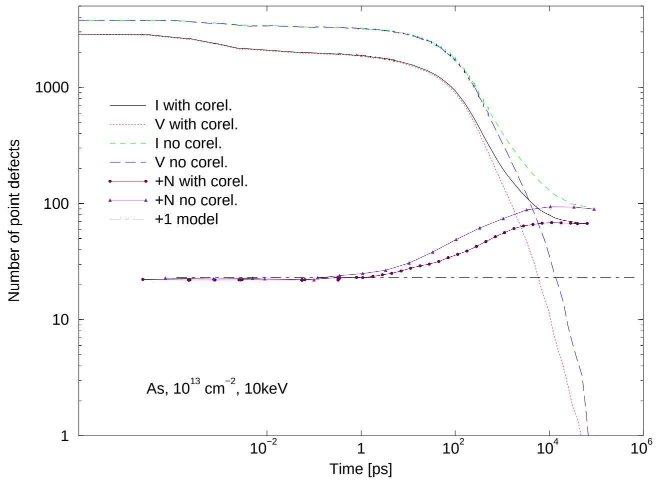

Figure 6: LMC simulations of the numbers of point defects remaining after a 10 keV, $10^{13}cm^{-2}$ As implant and subsequently annealing at 900°C [14]. The initial conditions are from either a Monte Carlo ion implant simulation [18] (with correl) or an initial random distribution of point defects with the same vertical profile (no correl). The initial correlation leads to a significant reduction in the number of interstitials remaining after the vacancies recombine (+3 versus +4).

vice properties. This is a particularly significant issue when extended defects are present since while a 50nm MOS structure may have hundreds of dopants, there may be only tens of dopant/defect clusters and one or two {311} defects.

CONCLUSIONS

We have illustrated some of the ways in which atomistic calculations can be effectively used to advance VLSI process modeling. There is clearly great potential for such methods to play an increasingly important role in advancing silicon technology.

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