A Simple Continuum Model for Simulation of Boron Interstitial Clusters based on Atomistic Calculations

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Abstract

Boron exhibits anomalous diffusion during the initial phases of ion implant annealing. Boron TED is characterized by enhanced tail diffusion coupled with an electrically inactive immobile peak. The immobile peak is due to clustering of boron in the presence of excess interstitials which also enhance boron diffusion in the tail region. In this paper we present a simple model for the formation of immobile boron clusters and associated point defect interactions derived based on atomistic calculations.

1. Introduction

Ion implantation is the primary means of dopant introduction in VLSI fabrication. It is well known that implantation introduces damage that on annealing leads to the phenomenon of transient enhanced diffusion (TED). Implantation introduces a large number of point defects orders of magnitude higher than the dopant concentration. These excess interstitials and vacancies recombine with each other during the initial stages of annealing. The remaining excess point defects also form extended defects, primarily $\{311\}$ defects for interstitials and boron interstitial clusters (BICs) for boron [1]. These defects interact with each other through changes in point defect and solute concentrations.

Under TED conditions, boron is found to be immobilized at concentrations well below solid solubility. This has been explained on the basis of the formation of boron interstitial clusters (BICs). Models using either a moment-based approach [2] or a discrete set of cluster compositions [3, 4] have been successfully used for modeling of boron interstitial clusters. A problem with both of these approaches is that they lead to complicated models with associated long simulation times and large sets of non-unique parameters.

In this paper we derive a simple single cluster model for BICs derived from a multi-cluster model based on *ab-initio* calculations performed at Lawrence Livermore National Labs [5]. Despite its simplicity, the model accurately describes boron clustering and anomalous diffusion over a wide range of experimental conditions. The resulting model can be easily incorporated into an industrial process simulator.

2. Multi-Cluster Models for Boron TED

Boron aggregation is a complicated process as there is a huge array of potential cluster compositions. In previous work, Lilak *et al.* [3] presented a boron clustering model based on the same calculations which we use in this work. Pelaz *et al.* [4] derived a similar model, but with a somewhat different parameter set. In both cases, they considered a large range of clusters as shown in Fig. 1(a), with an associated large set of continuity equations and parameters.

The model implemented in this work uses kinetic reactions that lead to the formation of clusters. For example, a substitutional boron can react with a silicon self interstitial to form an immobile BI which can further react with another interstitial to form a BI_2 cluster or with an interstitial boron (B_i) to give B_2I_2. For reactions of the form A + B $\Leftrightarrow$ C, the rate of formation of C is given by,

$$R = 4\pi r_{\text{cap}}(D_{\text{A}} + D_{\text{B}})(C_{\text{A}}C_{\text{B}} - \frac{C_{\text{C}}}{K_{\text{eq}}}) \tag{1}$$

where r_{cap} is the capture radius of the reaction and D and C represent diffusivity and concentration. Cluster energetics calculations from Zhu *et al.* [5] were used as the basis for the simulations, with 10 different clusters considered: BI, BI_2, B_2I, B_2I_2, B_3I, B_3I_2, B_4I_2, B_4I, B_2, B_3.

Our analysis of this system found that most of the clusters rapidly achieve dynamic equilibrium with the free boron and interstitial concentrations, suggesting the possibility of reducing the number of equations and parameters needed to describe the system. As shown in Fig. 1(b), except for B_3I and B_4I_2, all the clusters reach dynamic equilibrium with the B and I concentration within a very short time, while the two larger clusters are also in local dynamic equilibrium. At the same time, only a small subset of the clusters are ever present in significant numbers. From Fig. 2(a) we can see that BI_2 are the dominant cluster at very short times when the interstitial supersaturation is large. (Note that at such short times the B_3I and B_4I_2 clusters are negligible due to the slow formation of B_3I.) Once $\{311\}$ defects form, the interstitial concentration drops, and as can be seen from Fig. 2(b), the dominant species is B_3I.

3. Single-Cluster Model

Based on the above observations, we can simplify the system of immobile clusters from ten to just one continuity equation, that for B_3I, with the rate of formation given by

$$R_{\text{B}_3\text{I}} = k^r_{\text{B}_3\text{I}}(K_{\text{B}_3\text{I}}\text{C}_{\text{B}}^3\text{C}_{\text{I}} - \text{C}_{\text{B}_3\text{I}}) \tag{2}$$

In addition, we can also ignore the concentrations of small clusters other than BI_2, which we express in terms of the free boron and interstitial concentrations:

$$C_{BI_2} = K_{BI_2}C_BC_I^2 \tag{3}$$

We compared our simplified model to the full system and found that the results are virtually indistinguishable. A moment-based model characterized based on TEM results was used for $\{311\}$ defect kinetics [2]. Figs. 3(a) and (b) show examples of this comparison as well as to data from Intel [6] for TED at 800°C. Similar agreement was obtained at higher and lower temperatures (700 and 900°C) as well as for other implant doses.

4. Conclusions

In summary, we found that it is possible to develop a very simple model which accurately accounts for boron TED and clustering behavior. Based on analysis of cluster kinetics and energetics resulting from *ab-initio* calculations, we are able to match the results of a full multi-cluster model, while reducing the number of cluster continuity equations from ten to just one and the number of parameters from over twenty to only three. The resulting model clearly illuminates the critical processes involved in boron clustering.

References

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[6] M.D. Giles *et al.*, TED SIMS data from Intel Corporation.

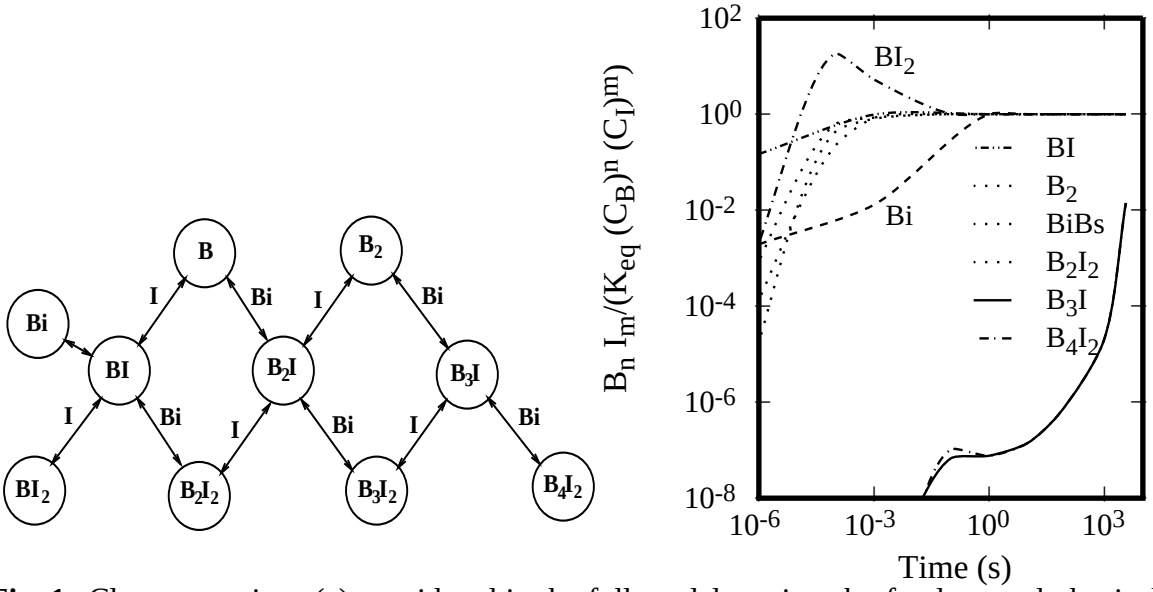

Fig. 1: Cluster reactions (a) considered in the full model as given by fundamental physical calculations [5]. Simulations (b) using the full cluster model of normalized cluster concentrations (relative to their equilibrium value) versus time for an 800°C anneal.

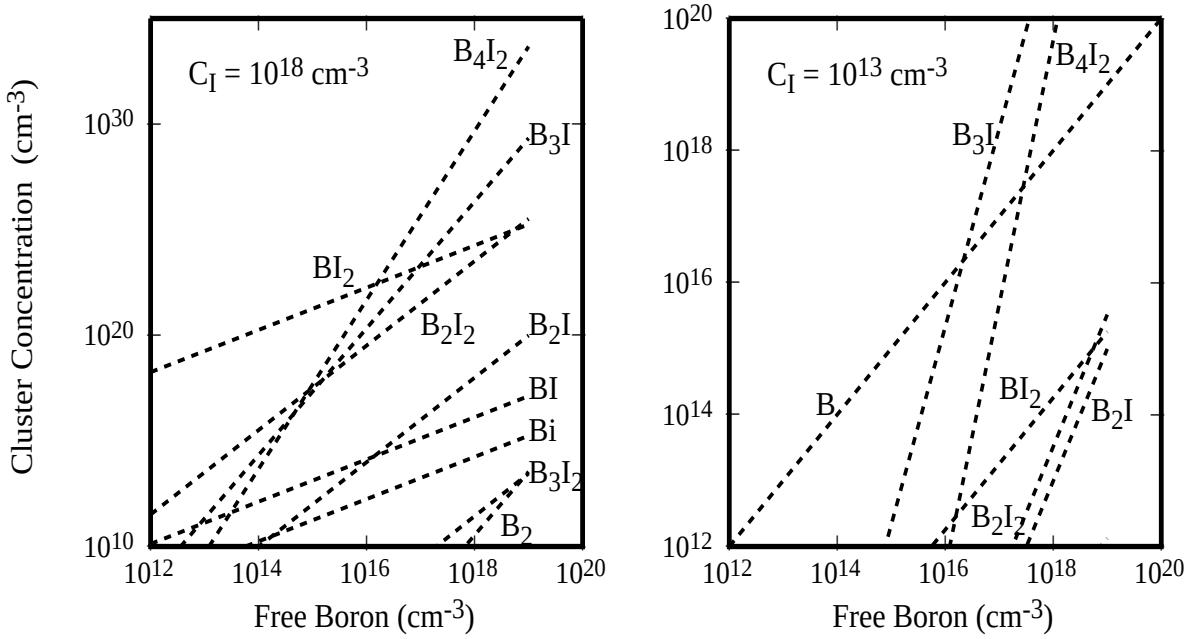

Fig. 2: Equilibrium cluster concentrations versus free boron concentration at 800°C for a free interstitial concentration of (a) 10^{18} cm^{-3} characteristic of very early stages of TED, and (b) 10^{13} cm^{-3} ($C_I/C_I^* \sim 10^4$) typical of TED conditions in the presence of {311} defects. Initially, BI_2 is the primary cluster and helps immobilize the boron as noted by Pelaz *et al.* [4], while B_3I is the primary cluster during most of the anneal.

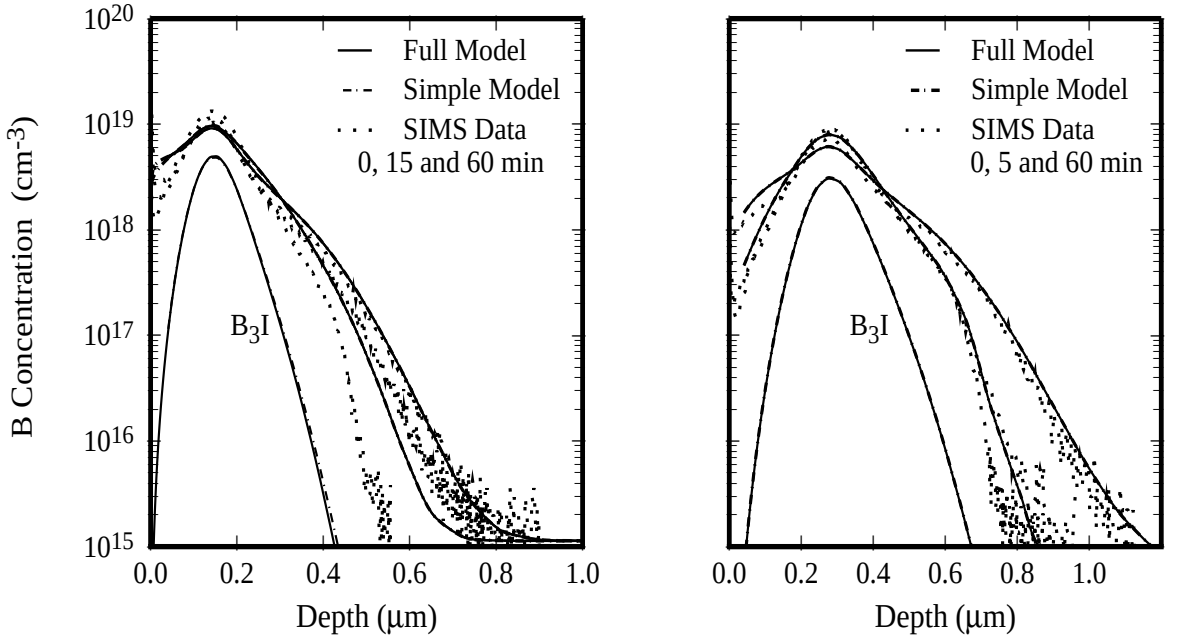

Fig. 3: Comparison of full model with the simplified model for (a) 40keV and (b) 80keV, 2×10^{14}cm^{-2} B implants annealed at 800°C for various times. Also shown for comparison are SIMS data from Intel [6]. Note that the full model and simple model show indistinguishable final profiles. The B_3I concentrations for the two models (shown after a 1 h anneal) are also nearly identical.