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Parallel Simulation of Ion Implantation for Multi-Component Targets Using Boltzmann Transport Equation

Shyh-Wei WANG and Shuang-Fa GUO*
Department of Electronic Engineering and Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan, R.O.C.

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A stepwise Boltzmann transport equation (BTE) simulation using non-uniform energy grid momentum matrix and exact nuclear scattering cross-section is successfully parallelized to simulate the ion implantation of multi-component targets. Assuming that the interactions of ion with different target atoms are independent, the scattering of ions with different components can be calculated concurrently by different processors. It is developed on CONVEX SPP-1000 and the software environment of parallel virtual machine (PVM) with a master-slave paradigm. A speedup of 3.3 has been obtained for the simulation of As ions implanted into AZ1350 ($C_{6.2}H_6O_1N_{0.15}S_{0.06}$) which is composed of five components. In addition, our new scheme gives better agreement with the experimental results for heavy ion implantation than the conventional method using a uniform energy grid and approximated scattering function.

KEYWORDS: parallel processing, multi-component target, exact nuclear scattering cross-section, non-uniform energy grid momentum matrix

1. Introduction

In the numerical solution of the Boltzmann transport equation (BTE),[1,2] the statistical momentum distribution function is represented by a matrix F_{ij} describing the number of ions moving with energy E_i in direction ϕ_j. To improve the simulated results, we have proposed a non-uniform energy grid momentum matrix and an exact nuclear scattering cross-section in the BTE calculations.[3] In this work, we will show that a parallelization skill is easily employed to simulate the ion implantation of multi-component targets because the interactions between ion and different target atoms can be assumed to be independent and the scattering of ions by different target atoms can be calculated concurrently by different processors. Our simulation program is parallelized in the environment of the Parallel Virtual Machine (PVM) software[4] on the platform of CONVEX SPP-1000 which owns 8 CPUs. A satisfactory speedup has been achieved over the conventional sequential approach.

In §2, we will briefly introduce the evaluation steps of the BTE method when the ion implantation is applied to multi-component targets. In §3, we will describe the parallelization procedures for multi-component target applications. In §4, we will discuss the speedup factor of parallelization and the simulation results, also compared to the experiment.

2. Boltzmann Transport Equation for Multi-Component Target

For ions moving through a multi-component target, the Boltzmann transport equation is[2]

$$\frac{\mathrm{d}}{F}(p)\mathrm{d}z = \sum_k N_k \int \left(\frac{F(\mathrm{p}')d\sigma_k(p' \rightarrow p)}{\cos\theta_{p'}} - \frac{F(p)d\sigma_k(p \rightarrow p')}{\cos\theta_p} \right) \quad (1)$$

where index k represents each component of target atoms, N_k is the number density of target atom k, $d\sigma_k(p \rightarrow p')$ is the total differential scattering cross-section of target atom k and $F(\mathrm{p}, z)dp$ is the number of ions having momentum in the region from p to $p + dp$ at a depth z from the sample surface. The right-hand side of eq. (1) contains terms for each type of atoms found in the target material. It is assumed that the probability of collision with a particular type of atoms is proportional to their stoichiometric abundance. For example, oxygen is encountered twice as frequent as silicon in SiO_2 target. In the numerical calculation, the momentum state of ions is given by a matrix F_{ij} which records the number of ions with energy E_i traveling in the direction ϕ_j. And also, a non-uniform energy grid is adopted in this work.[3]

The scattering cross-section $d\sigma$ consists of an elastic nuclear part $d\sigma_n$ and an inelastic electronic part $d\sigma_e$. The electronic stopping is usually modeled by the LSS theory.[5] The nuclear scattering cross-section is evaluated by the conventional one-parameter approximation proposed by Lindhard, Nielson and Schoitt (LNS).[6] It has been shown that a better agreement with the experiment results can be obtained by using the exact nuclear cross-section.[3] To obtain the differential nuclear scattering cross-section $2\pi pdp$, the impact parameter p is determined from the particle energy E and the scattering angel ϕ by solving the magic formula proposed by Biersack[7] iteratively. For each target component, a two-dimensional table of the impact parameter p as a function of the ion energy E and the scattering angle ϕ is constructed at the beginning. The desired value is interpolated from the table during the simulation process.[3]

3. Parallelization Procedures Using Multi-Processors

The BTE method takes a longer time than usual when it applies to multi-component target ion implantation simulations. Since every type atoms contained in the target material should be considered. There is one calculation pass for each type of atoms at a certain depth, *e.g.* one go for silicon and another for oxygen when the SiO_2 target is considered. It is important that the interactions between ions and different target atoms are assumed to be independent. The scattering of ions due to different sort target atoms can be traced by different processors simultaneously. This situation is very suitable to adopting the parallelization technique.

The parallelization program is developed in the environment of PVM[4] (Parallel Virtual Machine). The master/slave paradigm has been adopted to parallelize our simulation pro-

*E-mail address: sfguo@cc.nctu.edu.tw

gram. In this scheme, the master spawns and directs some slave programs which perform the computation. The data is exchanged between master and slaves by the message passing manner. This is accomplished by calling PVM subroutines. The flowchart of the parallelized program is shown in Fig. 1. The master program performs basic calculations and controls slaves to perform the two-dimensional tables for each type of atoms and forms the momentum matrix F and energy array E, and then, broadcasts them to all slaves. Each salve program is responsible for one type material atom and computes the changes of momentum matrix ΔF_k and an energy loss array ΔE_k at a certain depth then send back to master. The momentum matrix are calculated as[1)]

$$\Delta F_k = F N_k \Delta z \int_{T_1}^{T_2} d\sigma_{n_k} \Big/ \cos\theta \qquad (2)$$

where Δz is the step size, T_1 and T_2 are the minimum and maximum energy transfers between two different states, respectively. And the energy loss ΔE_k[1)]

$$\Delta E_k = N_k \Delta z \left(S_e + \int_0^{T_{\min}} T d\sigma_{n_k} \right) \Big/ \cos\theta \qquad (3)$$

where $T_{\min}$ is the minimum energy required to transfer a particle to the next state. After receiving all ΔF_k and ΔE_k from all slaves at a particular depth, master sums them up to get the overall variations ΔF and ΔE. Master redistributes F and E according ΔF and ΔE and get the stop profile N_s, then sends new F and E to slaves to proceed calculations at next depth. It is proceeded until most of the ions are removed from the momentum matrix due to scatterings.

4. Results and Discussion

The speed-up factors for parallelization of BTE are shown in Fig. 2. It contains As in SiO_2 and AZ1350 ($C_{6.2}H_6O_1N_{0.15}S_{0.06}$) for the energy range 10–500 keV. The slave number is equal to the contained element number, i.e., there are two slaves involved in the SiO_2 application while five slaves for AZ1350. Thus, from this figure, we can see that the speedup for SiO_2 is about 1.6 and 3.3 for AZ1350. The efficiency is about 80% for SiO_2 and drops to 66% for AZ1350. It is because that more communications are contained when more slaves are included, a lower parallelization efficiency is acquired for AZ1350.[8)]

In addition, we select cases for calculations in order to test the applicability of the new schemes presented above. In order to examine the effects of nuclear stopping power, heavy ions implanted into lighter substrate at low and intermediate energies are selected. So we perform the calculations of Au implanted in SiO_2 and Bi in AZ1350 in a 10–400 keV energy range. Comparisons of non-uniform grid using exact nuclear cross-section and conventional uniform grid using LNS approximation together with experiment data are also made.

The simulated range parameters, projected range R_p and straggling ΔR_p, using non-uniform grid with exact nuclear scattering cross-section and uniform energy grid with rational function approximation as well as the experiment results of Bethr *et al.*[9)] for Au ions implanted into SiO_2 in a 10–400 keV energy range are shown in Fig. 3. The SiO_2 density is assumed to be $2.3\,g/cm^{-3}$ [9)] and ZBL potential model is selected.[10)] We could see that the non-uniform grid with exact cross-section provides higher R_p and ΔR_p than uniform grid with LNS cross-section and a better agreement with the experiment is also achieved. The R_p and ΔR_p values of this work agree well with the experiment. Only for low energies (<70 keV), ΔR_p is slightly lower than the experimental data.

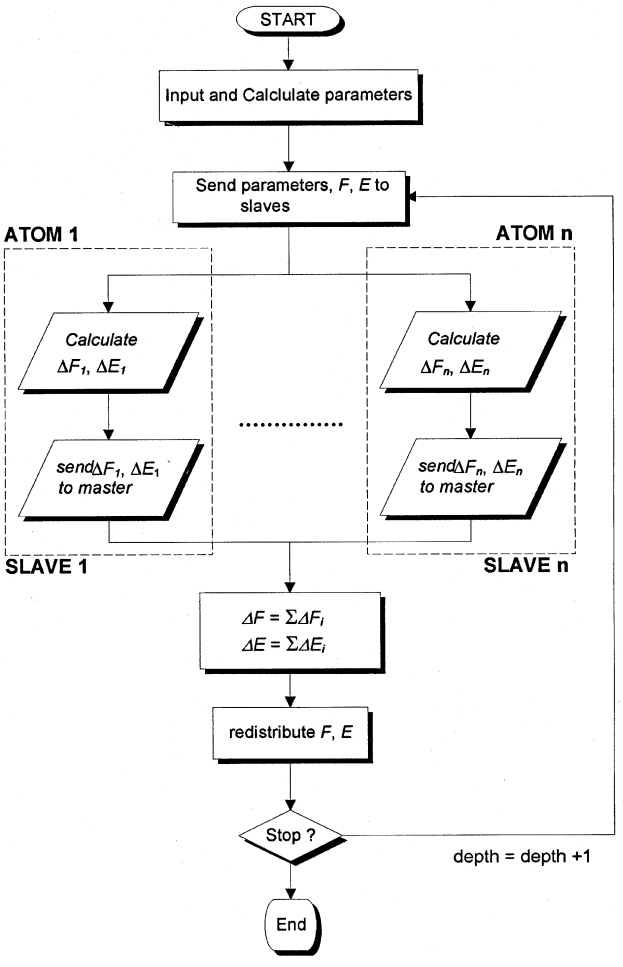

Fig. 1. Program flowchart of parallelized BTE for multi-component target implantation application.

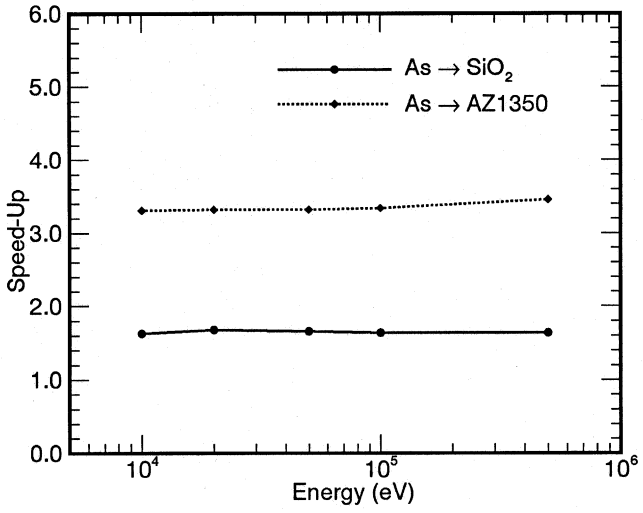

Fig. 2. Speedup factors of As in SiO_2 and AZ1350 for the energy range 10–500 keV.

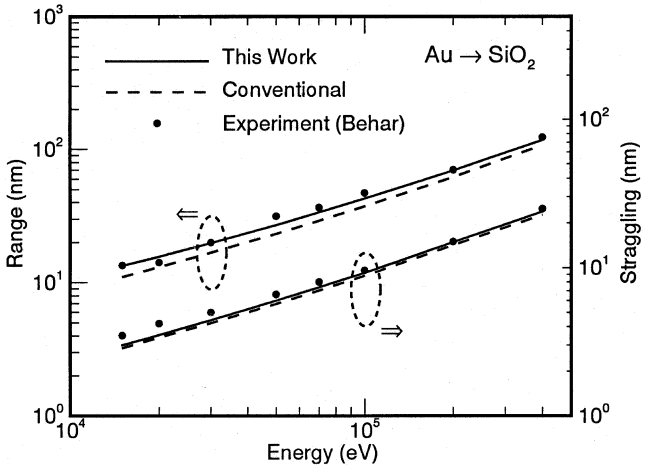

Fig. 3. Comparison of projected range and straggling for Au in SiO_2 obtained using new and conventional BTE together with the experimental data for various incident energy.

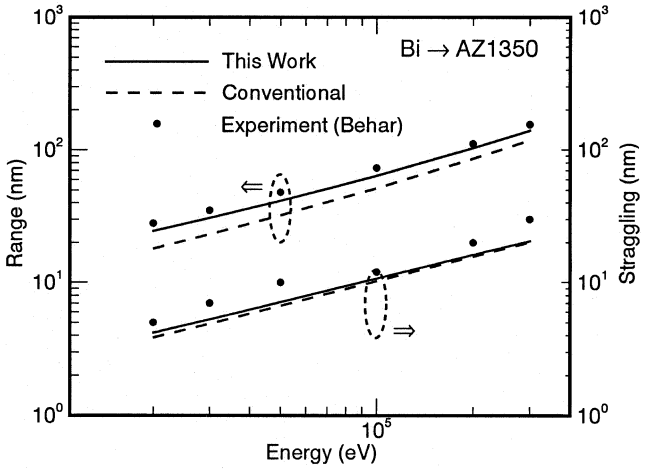

Fig. 4. Comparison of projected range and straggling for Bi in AZ1350 obtained using new and conventional BTE together with the experimental data for various incident energy.

The experimental R_p and ΔR_p as well as the BTE calculated parameters using different means for Bi implanted into AZ1350 in a 20–300 keV energy range are displayed in Fig. 4. We have assumed that the AZ1350 density is $\rho = 1.3\,\mathrm{g/cm^3}$, the composition is $C_{6.2}H_6O_1N_{0.15}S_{0.06}$[9] and ZBL potential model is selected. Once again, a better agreement with the experiment is also achieved by using the non-uniform grid together with exact cross-section. The R_p values of this work fit well with the experiment, but the experimental values exceed the calculated results significantly in concerning ΔR_p.

5. Conclusion

A parallel stepwise Boltzmann transport equation (BTE) using the non-uniform grid momentum matrix and exact cross-section evaluation is successfully built for multi-component target implantations. It could accelerate the evaluation procedures up to 3.3 times for AZ1350. Besides faster simulations, a more accurate simulation is also acquired with our new techniques. Our results shows that our new techniques fit the experimental data better than the conventional for the cases of Au in SiO_2 and Bi in AZ1350.

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