Fast Calculation of Material Radiation Damage by GPU Accelerated TRIM

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Abstract. An important function of TRIM is to research the radiation damage of ions implanted into materials. In this paper, GPU accelerated TRIM is developed for the fast calculation in study of material radiation bombarded by ions. The vacancies of iron induced by protons, alpha and carbon were simulated by GPU-TRIM. It reproduces the results well with SRIM2013. In the GPU test platform, TRIM achieves thousands of times the speed-up ratio.

1. Introduction
TRIM (Transport of Ions in Matter) is Monte Carlo (MC) computer code that calculates the interactions of energetic ions with amorphous targets [1]. It simulates the stopping and range of ions into matter using a quantum mechanical treatment of ion-atom collisions. It is widely used in the damage research of materials irradiated by low and medium energy particles [3,4]. GPU (Graphics Processing Unit) with the characteristics of high parallelism, low energy consumption and low cost, it has significant advantages in the computing tasks with high data parallelism, so it is highly concerned by experts and scholars [2]. The purpose of this work is to use GPU to accelerate the simulations process of TRIM and to realize a rapid assessment of material damage.

2. Physics and Methods
The Continuous Slowing Down Approximation (CSDA) method [1] is usually used to simulate the continuous collision process of charged particles in the coulomb field. Each particle is tracked along a path consisting of a number of steps. In each step, the rate of energy loss at every point along the track is assumed to be equal to the same as the stopping power. The total stopping cross-section of ions in target is divided into two parts: electronic stopping and nuclear stopping.

2.1. Electronic Stopping
The theoretical electronic energy loss of a proton in matter is calculated using the Lindhard local-density approximation [1]. For the convenience of the program, Ziegler et al. obtained the empirical formula of the electron stopping power of the proton though a large number of theoretical analysis and experimental data based on the Lindhard description framework. The helium stopping cross-sections are obtained by multiply the equivalent proton data by the He effective charge. We scaled proton stopping powers using Brandt-Kitagawa theory to obtain heavy ions stopping power [1].

2.2. Nuclear Stopping
Ziegler, Biersack and littmark (ZBl) use the universal potential and ‘scattering triangle method’ [1] to give a more accurate fitting formula in a large reduced energy range:
For incident ions, \( E_0 \) is the energy, \( \varepsilon \) is the reduced energy being calculated as:

\[
\varepsilon = \frac{32.53 \times M \times E_0}{Z_1 Z_2 (M_1 + M_2) (Z_1^{0.25} + Z_2^{0.25})}
\]

(2)

\( Z_1, Z_2 \) represent the atomic number of the incident particle and the target material, \( M_1, M_2 \) represent the atomic mass of the incident particle and the target material respectively. Then the reduced nuclear stopping energy is:

\[
S_n(\varepsilon) = \frac{\ln(1 + 1.1383 \varepsilon)}{2(\varepsilon + 0.01321 e^{0.1123\varepsilon} + 0.19593 e^{0.5})}
\]

\( \varepsilon \leq 30 \)  

(3)

\[
S_n(\varepsilon) = \frac{\ln(\varepsilon)}{2\varepsilon}  
\]

\( \varepsilon > 30 \)  

(4)

### 2.3. Kinchin-Pease Model

In quick TRIM, the modified Kinchin-Pease model is used to calculate the corresponding number of atomic displacements based on the formalism proposed by Norgett, Robinson, and Torrens [5] which is often referred to as the NRT model. The number of displacements \( N_v \) is derived from the following equation:

\[
N_v = \begin{cases} 
0 & E_{\nu} < E_d \\
1 & E_d \leq E_{\nu} < 2.5E_d \\
\frac{0.8E_{\nu}}{2E_d} & E_{\nu} \geq 2.5E_d 
\end{cases}
\]

(5)

Where, \( E_{\nu} \) is the damage energy and \( E_d \) is the threshold displacement energy.

### 2.4. GPU Parallel Algorithm

The structure of the GPU-TRIM based on NVIDIA’s CUDA architecture is illustrated in figure 1. The CPU (i.e., the host-side) controls the flow of the program to complete the variables initialization and parameters reading, the data copy between the CPU and the GPU, and the GPU (i.e., the device-side) completes the MC simulation.
Figure 1. GPU based TRIM parallel algorithm

Task partitioning is the key problem of parallel computing. As MC transport requires a large number of simulated particles and each particle is relatively independent, GPU-TRIM uses equal division. That is, a thread completes the transport of \( n / p \) particles, where \( n \) is the total number of particles, \( p \) is the number of threads started on GPU. The calculated particle number is increased by \( i = i + \text{blockDim.x} \times \text{gridDim.x} \), where \( i \) is the particle number. This implementation method can not only simulate enough particles, but also ensure the execution efficiency.

CUDA's built-in random number generator in parallel is used in GPU-TRIM. First, we use the \texttt{curand_init} function to initialize the random number generator, and then use the \texttt{curand_uniform} function to generate random numbers. The \texttt{curand_init} function sets up an initial state using the given seed, sequence number and offset. Because sequences generated by \texttt{curand_uniform} with the same seed and different sequence numbers will not have statistically correlated values, we make the \texttt{thread_id} as sequence to ensure that the random numbers are irrelevant.

3. Simulation Parameters and Results

Iron is one of the common nuclear materials elements, we choose it as the calibration material. For the code verification and comparison of acceleration efficiency, SRIM2013 was used to simulate the target damage distribution of protons in iron with the same scale, and the running times were also recorded. Protons, helium and carbon ions are typical particles in irradiation of nuclear materials, we select them as incident particles to simulate the vacancy creation distribution.

Table 1 shows the energy of three typical incident particles and the thickness parameters of the iron targets. The total energy of particle is set between 150KeV and 10MeV, and 100000 particles will be run in each case.

| Ion | Energy | 150KeV | 500KeV | 1MeV | 10MeV |
|-----|--------|--------|--------|------|-------|
| H   | 7.50E+03 | 2.80E+04 | 6.70E+04 | 3.00E+06 |
| He  | 6.00E+03 | 1.30E+04 | 2.25E+04 | 3.25E+05 |
| C   | 3.00E+03 | 5.80E+03 | 9.00E+03 | 4.50E+04 |
3.1. Target Vacancy Production

Figures 2, 3 and 4 show the vacancy distributions in iron target bombarded by various ions. The fast calculation mode which use Kinchin-Pease estimates is set in SRIM2013 calculation, and the number of particles is $1E + 5$. GPU-TRIM uses the same damage estimation model, and the number of particles sets $1E + 5$ and $1E + 7$. It can be seen the results of GPU-TRIM are in good agreement with SRIM2013. Among the comparisons, the case of carbon ion is the best, and the proton is second. The energy loss near the Bragg peak becomes obvious especially in the region of high energy. The nuclear energy straggling effect will become significant near the Bragg peak of high energy proton, the contrast error between GPU-TRIM and SRIM2013 is relatively large.

![Figure 2. Vacancy distributions in iron target bombarded by proton](image1)

![Figure 3. Vacancy distributions in iron target bombarded by helium](image2)
3.2. **Speedup Test of the GPU Algorithm**

NVIDIA Titan V is selected as the GPU-TRIM test platform in this work. SRIM2013 runs on ThinkPad-x1 notebook platform, equipped with standard voltage version CPU i7-8750h. Table 2 shows the comparison of the time consumption of SRIM2013 and GPU-TRIM in the calculation of 100000 particles. As can be seen, SRIM2013 has a computing time of between one hour to two hours, as GPU-TRIM computing time is compressed to only one second. The acceleration ratio reaches 5000-10000 times, that is because the TRIM random processes lie in the nuclear scattering and walk length determination, without nuclear reaction process, the time cost of each particle is almost equal. In a word, the TRIM is suitable for accelerating calculation by GPU.

**Table 2.** Comparisons of time consumption between SRIM2013 and GPU-TRIM to simulate $10^5$ particles

| Device                  | Ion | 150KeV   | 500KeV   | 1MeV     | 10MeV    |
|-------------------------|-----|----------|----------|----------|----------|
| Intel(R) Core(TM) i7-8750H | H   | 6841     | 9245     | 3861     | 5163     |
|                         | He  | 4923     | 4386     | 4443     | 6782     |
|                         | C   | 4322     | 5649     | 6547     | 10088    |
| NVIDIA TITAN V          | H   | 0.787    | 0.786    | 0.792    | 0.806    |
|                         | He  | 0.828    | 0.848    | 0.821    | 0.823    |
|                         | C   | 0.846    | 0.857    | 0.851    | 0.876    |
| Time Gain Factor (*10^3) |     | **5.1-8.7** | **5.2-11.8** | **4.9-7.7** | **6.4-11.5** |

### 4. Conclusion and Discussion

Based on the CUDA architecture of NVIDIA, the TRIM is developed on GPU. It can simulate tens of millions of ions transport histories interact with material in only few seconds because of its natural parallelism. The results of GPU-TRIM are in good agreement with those of SRIM2013. At present, the code can be used to fast analyze the radiation damage of materials. Next, we prepare to add ion full cascade transport mode to the code to improve the accuracy and versatility.

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**Figure 4.** Vacancy distributions in iron target bombarded by helium
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