Comparison of the stopping powers calculated by using rate equations with those by the Monte Carlo method

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Abstract. We calculate the stopping powers of H$_2$ for the Li projectiles by using rate equation and Monte Carlo methods. We treat the change in the charge number of the projectiles by using some atomic and molecular processes. The stopping powers by solving the rate equations agree well with those averaged by 100 trials by the use of the Monte Carlo method.

1. Introduction
Recent developments in ion source technique allow us to measure the track structure (the spatial distribution for the energy deposit from the ions to the target), the range, and the second particles such as electrons and ions more accurately [1, 2]. The energy deposit and the secondary particles, which are mainly caused by several atomic and molecular processes, play an important role for DNA damage [1], low dose damage [1], and surface modification for semiconductors [2].

In the ion stopping powers, which are indispensable for the study of the track structure, the charge number of the ions plays an important role [3, 4]. The charge numbers are mainly determined by some atomic and molecular processes such as charge transfer (A$^{z+}$ + B $\rightarrow$ A$^{(z-1)+}$ + B$^+$), and electron loss of the projectile (A$^{z+}$ + B $\rightarrow$ A$^{(z+1)+}$ + B + e$^-$), where A$^{z+}$, B, and e$^-$ are a heavy particle, a target molecule, and an electron, respectively, and z is the charge number of the particle [5, 6]. For the calculation of the stopping powers as a function of times or invasion lengths, the population of each charge number of the projectile should be treated. However, in the calculation of the track structure and the range of heavy particle radiations, there are only a few studies [5-10], which have treated heavy particles with an energy lower than 300 keV/u [7,11]. Furthermore, no paper has treated particles heavier than the a particle and the excited states of the projectiles as far as we know. We calculated stopping powers of H$_2$ for Li ions by using rate equations [8], which can treat the population of the electronic states of a projectile. On the other hand, we have tried to solve the stopping powers by using the Monte Carlo method [9] because the Monte Carlo method is more suitable for parallel super computers than that for the direct calculation of rate equations. In this paper, we compare the stopping powers calculated by solving rate equations with those by using the Monte Carlo method.

2. Method of calculations
For atomic and molecular processes, we consider impact ionization (A$^{z+}$ + B $\rightarrow$ A$^{z+}$ + B$^+$ + e$^-$), impact excitation (A$^{z+}$ + B $\rightarrow$ A$^{z+}$ + B$^+$), charge transfer (A$^{z+}$ + B $\rightarrow$ A$^{(z-1)+}$ + B$^+$), and electron loss of the
projectile \((A^{z+} + B \rightarrow A^{(z+1)+} + B + e^-)\), where \(B^*\) expresses the excited state of \(B\). Here, we do not treat the excited states of \(Li\) ions because the excited states of \(Li\) ions have only a little effect on the stopping powers \([8, 9]\). Though excitation processes of the projectiles may be important as pointed out in Ref. \([12]\), they are not treated here because there are no available data. The energy losses given by the impact ionization and electron loss of the projectile are the sum of the bound energy of the target and the initial energy of the secondary electron. We employ the Rudd model \([13]\) for the energy distribution of the secondary electrons.

By treating these atomic and molecular processes, we calculate electronic stopping powers for the \(Li\) projectiles as a function of invasion lengths of the projectile by using the rate equations and Monte Carlo method. For the rate equation method, we use the same method as that given in Ref. \([5-7]\). Namely, we solve the population of the various charge numbers by the following rate equations:

\[
\frac{dP_k}{dr} = -\alpha_k P_k + \sum_{\alpha \rightarrow k} \beta_{mk} P_m,
\]

where \(P_k\), \(r\), \(\alpha_k\) and \(b_{mk}\) are the population, penetration length, decay constant in the \(k\)th state, and the transition rate from the \(m\) state to \(k\) state, respectively. Then, the stopping powers are given by

\[
S_p = \sum \sum P_k \sigma_p E_{kp} N_t,
\]

where \(S_p\), \(\sigma_p\), \(E_{kp}\), and \(N_t\) are the stopping power, the cross sections of process \(p\), the energy loss caused by process \(p\) for state \(k\), and the target density, respectively. On the other hand, for the Monte Carlo method, the following procedures are executed. (i) Suppose that the step size of penetration length is \(dr\), then, a bare (no electron) ion with an energy of 2 MeV/u enters the target at \(r=0\). (ii) The value of \(r\) increases by \(dr\) and the nuclear stopping power is calculated, where an impact parameter of the projectiles with the target is given randomly. (iii) In order to treat the processes equally, we randomly choose an atomic and molecular process and (iv) calculate the probability for the occurrence of this process, that is, \(s_p N_t dr\). (v) Only when this probability is larger than a random number, we judge that this process takes place. Then, the energy of the projectile, the charge number, and the electronic states of ions are changed according to this process. (vi) When this process does not take place, we choose another process and execute the procedures (iv) and (v). (vii) Until one process occurs or all processes do not take place, the procedures (iii)-(vi) are executed. (viii) We reiterate the procedures (ii) - (vii) until the energies of the projectile become smaller than 10 keV/u. We define one trial for the calculation of the procedures (i) - (viii). We have executed a lot of trials and calculate the stopping powers averaged over the number of trials.

**Figure 1.** Comparison of the stopping powers \((S_p)\) vs. penetration lengths \((r)\) by solving rate equation and the Monte Carlo method. For the Monte Carlo method, the numbers of the trials \((N_t)\) are (a) 1 and (b) 100.
3. Results and discussions
We treat a target of H$_2$ molecules with a density of 10$^{22}$/cm$^3$ and Li$^{3+}$ projectiles with an energy of 2 MeV/u. The energy and the charge number of the projectile have been changed as a function of $r$. Figures 1 (a) and (b) show the comparison of stopping power ($S_p$) vs. $r$ by solving the rate equations with those averaged by use of the Monte Carlo method for $N_t = 1, 100$, respectively, where $N_t$ is a number of trails. For $N_t = 1$, there is a big difference at the peak position of the stopping powers. As $N_t$ increases, both stopping powers agree better. We judge that the stopping powers converge when we take $N_t = 100$.

The rate equation method is based on a population of the charge numbers for the projectile, that is, the stopping powers for a single projectile, which has integer values for the charge numbers, is not calculated. On the other hand, in the Monte Carlo method, the change of the charge number for a single projectile is treated. However, there are some doubts for this method because the calculation depends on random numbers, that is, it includes the element of a gamble. Namely, both methods have disadvantages, which lead to doubts about the validity of the results. Therefore, the agreement between the results by using the two methods removes such doubts. In our future plans, we will calculate the collisional scattering of projectiles with a target and study the track structure. Since we will use a Monte-Carlo method for the calculation of the collisional scattering, it is useful to develop the Monte-Carlo code for the calculation of stopping powers treated in this paper.

4. Conclusions
We compare the stopping powers calculated by using rate equations with those by the Monte Carlo method. When the number of trials for the Monte Carlo method becomes 100, the stopping powers converge.

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