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COLLISION BETWEEN TWO HYDROGEN ATOMS

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Abstract. The interaction in a collision between two hydrogen atoms is studied using the 4-body classical trajectory Monte Carlo method. We present the total cross sections for the dominant channels, namely for single ionization of the target, and ionization of the projectile, resulting from pure ionization and also from electron transfer (capture or loss) processes. We present our cross sections in the projectile energy range between 20 keV and 100 keV and compared with them of previously obtained experimental and theoretical results.

1. EXPERMENTS

1.1. INTRODUCTION

The classical-trajectory Monte Carlo (CTMC) method is largely employed in collision physics from low to high projectile energies to determine the excitation, charge exchange and ionization cross sections (Reinhold and Falcón 1986). The CTMC method has been successful in dealing with the ionization processes in ion–atom collisions (Schultz and Olson 1988, Schultz 1989, Schultz, Reinhold et al. 1989, Schultz, Meng et al. 1992, Sparrow and Olson 1994, Tőkési, DuBois et al. 2014, Tökési, Wang et al. 1994). One of its main advantages is that all interactions among the particles can be taken into account exactly during the collision within the framework of the classical dynamics. The model is based on the numerical integration of the classical equations of motions for the investigated system.

For the case of the collision between two hydrogen atoms all the interactions can be exactly taken into account (Tőkési, DuBois et al. 2014). Here we can take the advantage of the classical treatment that in principle we do not have any

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theoretical limit for the number of particles. We can follow all particle trajectories during the collision with the restriction of the classical dynamics.

In this work, we present the total cross sections for the dominant channels, namely for single ionization of the target, and ionization of the projectile, resulting from pure ionization and from two-step processes of electron transfer (capture or loss). Furthermore, we present cross sections for the complete break of the system resulting in the final channel for free particles

Calculations were carried out at low energies, relevant to the interest of the fusion research. We present our cross sections in the projectile energy range between 20 keV and 100 keV and compared with them of previously obtained experimental and theoretical results.

1.2. SIMULATION

In our model the four particles (target nucleus, target electron and projectile electron, and projectile nucleus) are characterized by their masses and charges. Let us denote the projectile nucleus by P, the projectile electron by P_e, the target nucleus by T and the target electron by T_e. The electron-electron interaction is explicitly included in our 4-body calculation. At the time ($t = -\infty$) we consider four particles as two separate atoms, consisting of the projectile system (P, P_e) labelled as particles (1, 2), and the target system (T, T_e) labelled as particles (3, 4) (Fig. 1). Initially, both the projectile (P, P_e) and the target (T, T_e) are in the ground state. We use Coulomb potential for describing all interactions. Figure 1 shows the relative position vectors of the four-body collision system.

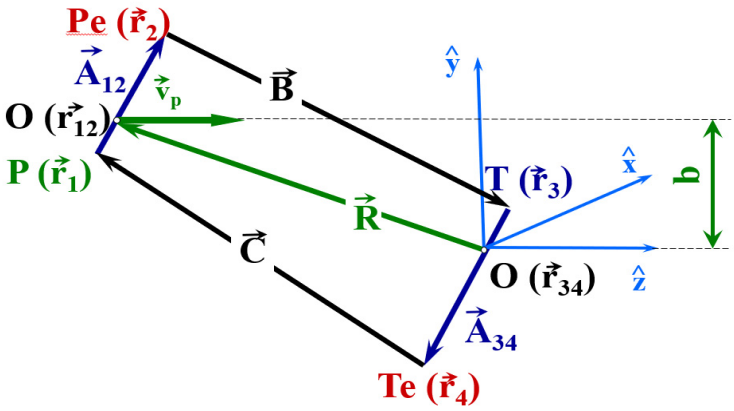

Figure 1: The relative position vectors of the particles involved in 4-body collisions.

In the present CTMC simulations, Newton's classical nonrelativistic equations of motions for four-body system are solved numerically for a statistically large

number of trajectories with initial conditions determined pseudorandomly. The Newton's equations can be written as:

$$m_i \frac{dr_i^2}{dt^2} = \sum_{i \neq j} Z_i Z_j \frac{|r_i - r_j|}{|r_i - r_j|^3} \quad (i, j = 1,2,3,4), \tag{1}$$

where $\mathbf{m_i}$, $\mathbf{r_i}$, and $\mathbf{Z_i}$ denote the mass, the position vector, and the charge of the ith particle, respectively.

The initial conditions are chosen, at relatively large internuclear distances between the projectile and target atoms (**R**, in Fig. l), randomly from an ensemble approximating the quantum mechanical phase space distribution for two separate atoms. After numerically integrating to large distances from the collision center the exit channels are determined according to the relative two body energies.

1.3. RESULT

To study the collision between two ground state hydrogen atoms we performed a classical simulation with an ensemble of 5×10^5 primary trajectories for each energies. In this work we focus on the investigation of the ionization channels.

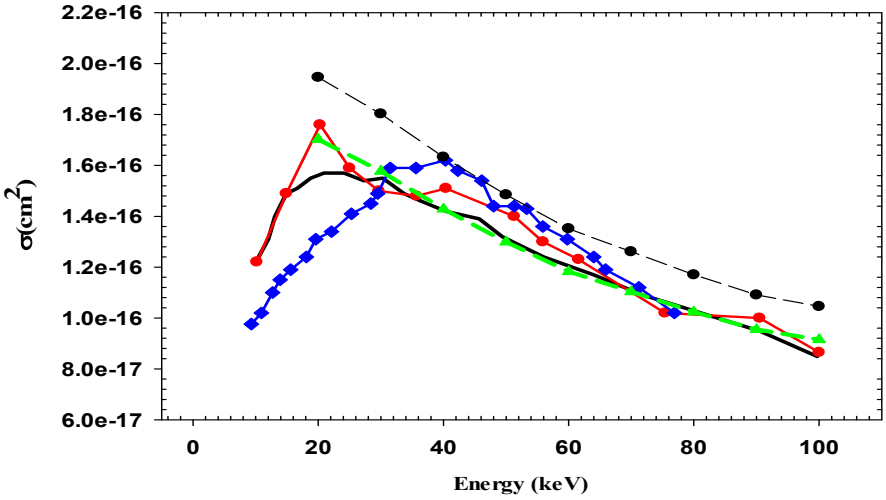

Figure 2: Target ionization cross sections as a function of projectile impact energy. Green dash-line: present CTMC results for H+H collision multiply by 1.75; Black circle with dash-line: present CTMC results for H+H collision multiply by 2; red circle with solid line: experimental data of $H+H_2$ by Solov'ev et al. 1962; blue diamond with solid line: Schwirzke 1960.

Figure 2 shows the energy dependence cross sections of ionization of atomic and molecular hydrogen by atomic hydrogen projectiles impact. Earlier data are available only for ionization of molecular hydrogen; they were obtained by Solov'ev (Solov'ev, Il'in et al. 1962) and Schwirzke (Schwirzke 1960). The ionization cross section for hydrogen molecule is greater than for hydrogen atom target. However the multiplication factor is not 2 as at first we can expect, but 1.75. So the ionization cross section for molecular hydrogen cannot be obtained by simply multiply the cross sections calculated from atomic hydrogen target. The reduction maybe attributed also to the screening of the projectile electron.

Acknowleedgments

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