# Classical simulation of the collision between $Be^{4+}$ and H

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**Synopsis** The interaction between $Be^{4+}$ and hydrogen atom is studied using the 3-body classical trajectory Monte Carlo method. We present total cross sections for target ionization, target excitation, and electron capture to the projectile bound state. Calculations were carried out in the projectile energy range between 100 and 500 keV/amu. As a test we performed the simulations assuming the H(1s) target. We present also simulation results when the target atom are in excited states, H(n>1), before the collsions. Our present results are compared with available previous data.

The currently used energy production methods will not be able to satisfy the energy needs of humanity in the long run. One of the best solutions in future would be the implementation of fusion power plants where Beryllium is a key element as the armor material of the first wall of the International Thermonuclear Experimental Reactor (ITER) [1]. Chemical and physical erosion of the first wall releases beryllium atoms and several molecular species, which eventually lead to the presence of fully stripped beryllium ions in the plasma core. Beryllium is attractive as a plasma facing reactor material because of its low atomic number (i.e. low potential for radiative plasma power losses), excellent gettering properties with respect to oxygen (unavoidably present in any fusion plasma) and adequate thermo-mechanical and erosion properties when exposed to plasma energy and particle fluxes. The inelastic collision processes between $Be^{q+}$ ions and H are particularly important when energetic neutral hydrogen are injected into the plasma for heating and diagnostic purposes [2]. Along this line, in this work, the interaction between $Be^{4+}$ and hydrogen atom is studied using the 3-body classical trajectory Monte Carlo method (CTMC) in the projectile energy range between 100 and 500 keV/amu.

In the last two decades there was a great revival of the CTMC calculations applied in atomic collisions involving three or more particles. This approximation seems to be useful in treating atomic collisions where the quantum mechanical ones become very complicated or unfeasible [3-6]. One of the advantages of the CTMC method is that many-body interactions are exactly taken into account during the collisions on a classical level.

The CTMC method is a non-perturbative methods, where classical equations of motions are solved numerically. In the present work the CTMC simulations were made in the three-body approximation. The three particles (target nucleus, target electron and projectile) are characterized by their masses and charges.

For the description of the interaction among the particles a Coulomb potential was used.

We present total cross sections for target ionization (see Eq. 1), target excitation (see Eq. 2) and electron capture to the projectile bound state (see Eq. 3).

$$Be^{4+} + H \rightarrow Be^{4+} + H^{+} + e^{-} \quad (1)$$

$$Be^{4+} + H \rightarrow Be^{4+} + H^{*} \quad (2)$$

$$Be^{4+} + H \rightarrow Be^{3+}(nl) + H^{+} \quad (3)$$

We present simulation results when the target atoms are either in the ground or in excited states, H(n>1), before the collsions. Our present results are compared with available previous data.

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