Calculation of ion stopping in dense plasma by the Monte-Carlo method

IOP Conf. Series: Journal of Physics: Conf. Series **946** (2018) 012014 doi:10.1088/1742-6596/946/1/012014

Calculation of ion stopping in dense plasma by the Monte-Carlo method

S K Kodanova[1], T S Ramazanov[1], M K Issanova[1], N Kh Bastykova[1], R I Golyatina[2] and S A Maiorov[2]

[1] Research Institute of Experimental and Theoretical Physics of the Al-Farabi Kazakh National University, al-Farabi Avenue 71, Almaty 050040, Kazakhstan
[2] Prokhorov General Physics Institute of the Russian Academy of Sciences, Vavilova 38, Moscow 119991, Russia

E-mail: bastykova_nuriya@physics.kz

Abstract. In this paper, the Monte-Carlo method was used to simulate ion trajectories in dense plasma of inertial confinement fusion. The results of computer simulation are numerical data on the dynamic characteristics, such as energy loss, penetration depth, the effective range of particles, stopping and straggling. By the results of the work the program of three-dimensional visualization of ion trajectories in dense plasma of inertial confinement fusion was developed.

1. Introduction

Recently, a large number of theoretical and experimental studies of the physical processes that determine the construction of a thermonuclear target and the required parameters of a future driver carried out [1–9]. The calculation of thermonuclear target parameters for heavy ion inertial fusion requires adequate quantitative description of heavy ion interaction with the dense plasma in a wide range of parameters. Therefore, in order to know the properties of the dense plasma under different conditions, the most attractive way is a computer experiment. Computer simulation can answer many important questions, which are to be known to use the dense plasma.

Nowadays, there are various programs which allow us to carry out simulation of ion implantation process in solids without experiments. Simulation has some error and is not able to fully replace real experiments, but its results provide invaluable assistance in future research. The best-known programs are the SRIM (the stopping and range of ions in matter) [10] and Geant4 [11].

The main energy contribution of heavy ion beams in different types of fusion targets occurs in dense high-temperature plasma. Therefore, knowledge of free paths and energy input profiles of fast and heavy charged particles in the plasma will help to determine the characteristics of the thermonuclear target most precisely.

In this paper, the Monte-Carlo method is used for simulation of ion trajectories in dense plasma of inertial confinement fusion. The main advantage of calculations by the Monte-Carlo method is that they allows us to take into account any physical process directly, for example, local and non-local inelastic energy losses, binding energy between atoms, replacing collision, etc. Moreover, it is possible to obtain accurate solutions for multi-target and multi-layered complex geometry, which allows us to simulate actual interactions with the plasma ion beam. The paper

considers the interaction of xenon ions in copper and beryllium, and iron ions in the mixture of deuterium, tritium and hydrogen at different energies.

The results of computer simulation are numerical data on the dynamic characteristics, such as energy loss, penetration depth, the effective range of particles, stopping and straggling. By the results of the work the program of three-dimensional visualization of ion trajectories in dense plasma of inertial confinement fusion was developed.

2. Formulation of the problem

Interaction of energetic ions with atoms, ions and electrons of the target is very complicated. The plasma ion beam eZ_1 charge interacts with the plasma ions with a charge eZ_2 and this interaction is described by the Coulomb potential

$$U(r_{12}) = \frac{e^2 Z_1 Z_2}{r_{12}}. \tag{1}$$

Electrons and ions of the plasma is screened the Coulomb particles interacts and to take into account of the screening used Yukawa potential

$$U(r_{12}) = \frac{e^2 Z_1 Z_2}{r_{12}} \exp(-r_{12}/r_{\text{Debye}}), \tag{2}$$

where r_{Debye} the radius of the Debye–Hückel determines the characteristic dimension of interaction between charges.

The ion polarizes atoms by its electric field and interacts with induced dipoles. The potential energy of this interaction at distances greater than the diameter of the atom and smaller than the average interatomic distance $N^{-1/3}$ is equal to

$$U(r_{12}) = \frac{\alpha \text{Ry} a_0^4}{r_{12}^4}, \tag{3}$$

where r_{12} is the distance between the atom and ion, $\alpha = \alpha_0/a_0^3$, α_0 is atomic polarizability, $a_0 = 0.529 \times 10^{-8}$ cm is the Bohr radius, Ry = 13.6 eV is the Rydberg constant, and N is the atom number density. The polarization collision cross section is $\sigma_{\text{pol}} \sim 1/v_{12}$, and the model of a constant ion collision frequency (independent of velocity) is applicable for the determination of ion mobility in the case of prevalence of polarization collisions. Obviously, at large distances effects of shielding are important, whereas at small distances the linear approximation for polarization does not work. However, the polarization approximation gives a very good accuracy for the ion mobility coefficients in the non-parent gas.

3. Algorithm for simulating ion–atom collisions

The ion–atom collisions in the process of ion motion were simulated by integrating the equations of ion motion. At each time step, the ion–atom collision was simulated by the Monte Carlo (MC) method. The main parts and elements of the algorithm developed for simulating the ion–atom collision are as follows:

(i) in accordance with the probability of the collision, the velocities of the particles and the impact parameter of the collision are chosen randomly in the center-of-mass frame of colliding particles;

(ii) in the center-of-mass system of moving particles with the polarization interaction potential (3) one determines the closest approach $r_{\min}$, the relative particle velocity $v_{12}(r_{\min})$ at the point of closest approach, and the scattering angle χ [12];

(iii) if $r_{\min} > d_{\text{gas}}$, here d_{gas} is effective diameter of an atom, the ion and atom velocities decline by the angle χ;

(iv) if $r_{\min} < d_{\text{gas}}$, the ion and atom velocities are recalculated according to the law of elastic sphere collision, the closest approach is assumed to be $r_{\min} = d_{\text{gas}}$, and the relative particle velocity is determined at the point of closest approach $v_{12}(r_{\min})$;

(v) the resonant charge exchange cross section $\sigma_{\text{res}}(v_{12}(r_{\min}))$ is determined for the relative particle velocity $v_{12}(r_{\min})$ at the point of closest approach;

(vi) for the closest approach $r_{\min} < r_{\text{ct}} = [2\sigma_{\text{res}}(v_{12}(r_{\min}))/\pi]^{1/2}$, the ion and atom velocities change with probability of 1/2;

(vii) the velocities are recalculated in the laboratory frame and statistics for various collision characteristics is accumulated.

The algorithm developed here reproduces the familiar solution to the Boltzmann kinetic equation for the drift motion of charged solid spheres [13], the ion mobility in the weak field limit [14] and known theoretical results on the kinetics of a collision between elastic spheres [15] and experimentally measured coefficients of ion mobility in gas.

In addition to ion–atom collisions in the plasma plays an important role stopping of ion by an electron gas and the collision with the ions. The above algorithm was used in considering the drift of ions in the gas at moderate electric field $E/N < 10000$ Td (1 Td $= 10^{-21}$ V m^2).

In this paper to simulate the collision of energetic ions is used the following modification with the atoms of the above-described algorithm of the extraordinary complexity of the process of collision of many-electron systems, with a collision energy of greater ionization potential. The radius of the rigid sphere was chosen depending on the collision energy by the following formula:

$$d_{\text{gas}}(\varepsilon_{12}) = d_{\text{gas}}(0)/(1 + \varepsilon_{12}/I). \tag{4}$$

here $d_{\text{gas}}(0)$ is gas-kinetic diameter of an atom, ε_{12} is energy collisions, determines the relative velocity and reduced mass, I is ionization potential. Equation (4) is proposed based on the dimension theory and asymptotic analysis. Despite its simplicity, it allows in many cases to obtain not only qualitatively reasonable results, but also quite good agreement with the experimental data. The situation is a definite analogy with the well-known case of Coulomb collisions when using the introduction of the Coulomb logarithm of many-body problem is reduced to instantaneous pair collisions of hard spheres, the diameter of which depends on the velocity.

4. Calculation results and discussion

Figure 1 shows the results of calculations of the stopping characteristics of singly charged iron ions with an initial energy of 30 keV in hydrogen isotopes with a temperature of 500 K: the trajectory of iron ions in the hydrogen isotope–protium, deuterium and tritium. The figure also shows the stopping range in the longitudinal direction of the R and the dispersion in the longitudinal and transverse directions. Analysis of these figures suggests a strong dependence of the longitudinal characteristics of the reduced mass.

Figure 2 shows the calculated the stopping of xenon ions in copper with initial energies of 5, 15 and 30 keV. The dependence of the energy of the ions range well known with experimental data xenon in copper [16]. Another interesting feature of these results is the effect of the anisotropic diffusion-dispersion stopped ions (straggling) in the longitudinal direction along the beam direction is approximately two times higher than in the transverse direction. A more detailed analysis of this phenomenon will be performed in the further work.

Figure 3 shows the trajectories of the xenon ions in the copper obtained from SRIM for different ranges of initial energy. Our calculations using the Monte-Carlo methods have a good agreement in comparison with the SRIM results, which confirms the correctness of our calculations and allows calculating other dynamic characteristics.

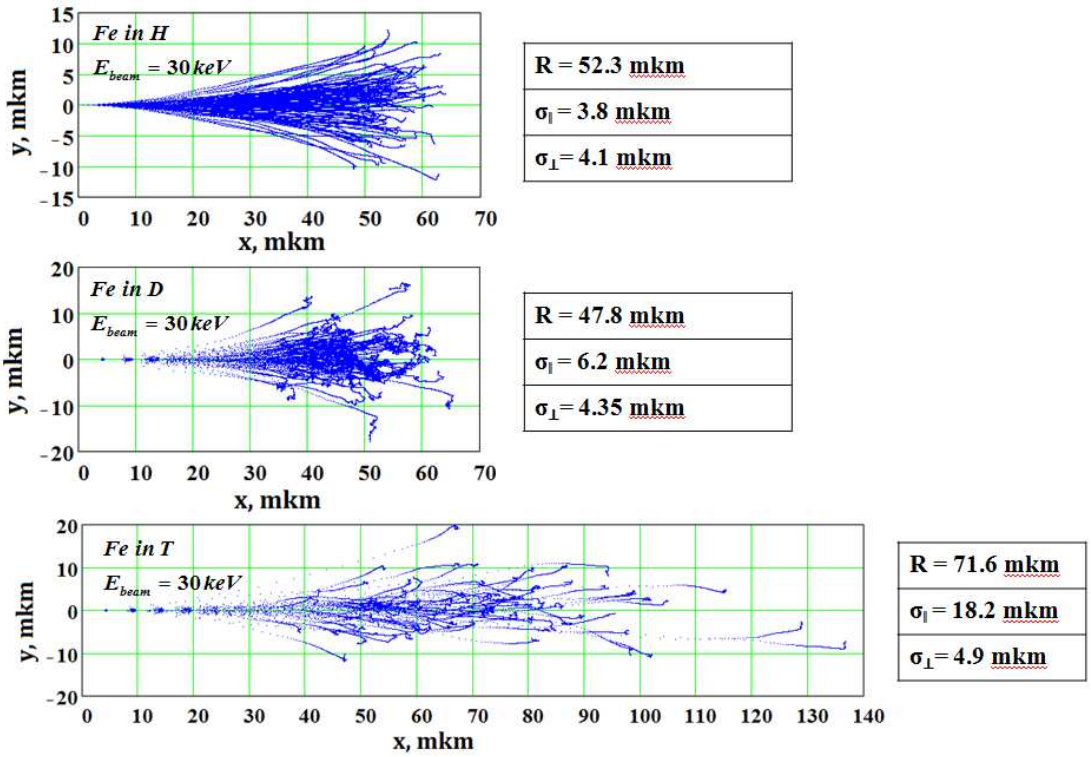

Figure 1. The trajectories of iron ions with an initial energy of 30 keV hydrogen isotopes: (from the top) protium, (in the middle) deuterium and (from the bottom) tritium. The figure also shows the stopping range and the dispersion in the longitudinal and transverse directions.

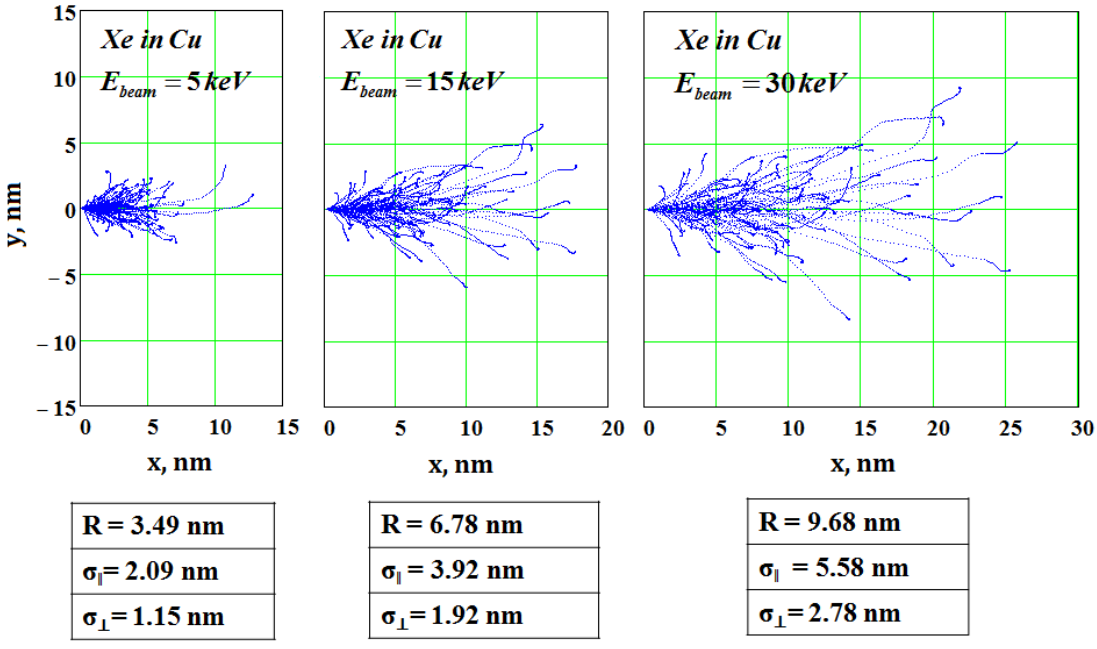

Figure 2. The trajectories of the xenon ions in the copper with an initial energy of (from the left) 5, (in the middle) 15 and (from the right) 30 keV. Figure shows the stopping range of the xenon ions depending on the energy in copper.

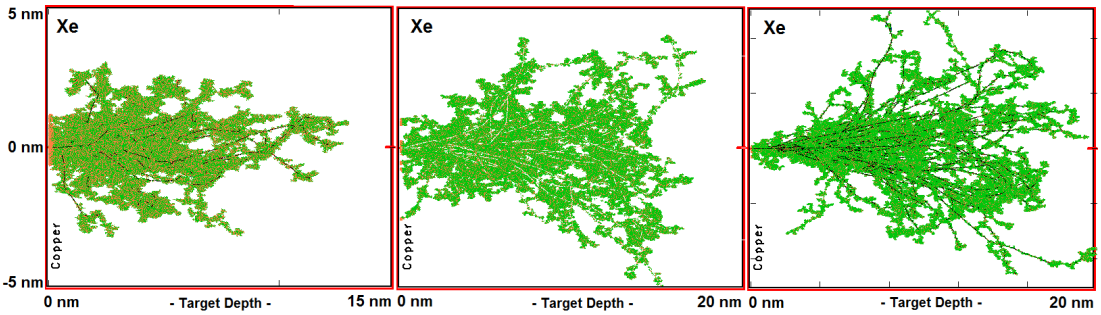

Figure 3. Results obtained from SRIM: The trajectories of the xenon ions in the copper with an initial energy of 5 (on the left), 15 (in the middle) and 30 keV (on the right).

5. Conclusion

The paper considers the interaction of xenon ions in copper and beryllium, and iron ions in the mixture of deuterium, tritium and hydrogen at different energies. Heavy ion inertial confinement fusion is more perspective as has more efficient energy absorption, higher pulse repetition rate and higher energy per pulse. The realization of the idea of controlled thermonuclear fusion with inertial confinement primarily requires a reliable estimation of physical characteristics of dense plasma. Therefore, for adequate description of processes occurring in dense plasma, reliable data on collision, transport, dynamic and other characteristics of the system are required. In the practical applications, the obtained results will allow scientists to estimate parameters of experiments on nuclear fusion with inertial confinement and thus can bring us closer to the creation of power facilities based on inertial confinement fusion.

Acknowledgments

This work has been supported by the Ministry of Education and Science of the Republic of Kazakhstan under grant No. 3083/GF4 (2017) aimed to develop informational-program package for modeling and visualization of dense plasma properties in inertial confinement fusion.

References

[1] Dharma-Wardana M W C and Perrot F 1998 *Phys. Rev.* E **58** 3705–18
[2] Gericke D O, Murillo M S and Schlanges M 2002 *Phys. Rev. Lett.* **65** 036418
[3] Brown L S, Preston D L and Singleton Jr R L 2005 *Phys. Rep.* **410** 237–333
[4] Glosli J N, Graziani F R, More R M, Murillo M S, Streitz F H, Surh M P, Benedict L X, Hau-Riege S, Langdon A B and London R A 2008 *Phys. Rev.* E **78** 025401
[5] Dimonte G and Daligault J 2008 *Phys. Rev. Lett.* **101** 135001
[6] Singleton R L 2008 *Phys. Plasmas* **15** 056302
[7] Issanova M K, Kodanova S K, Ramazanov T S, Bastykova N K, Moldabekov Z A and Meister C V 2016 *Laser Part. Beams* **34** 457–66
[8] Issanova M K, Kodanova S K, Ramazanov T S and Hoffmann D H H 2016 *Contrib. Plasma Phys.* **56** 425–31
[9] Hoffmann D H H *et al* 2005 *Laser Part. Beams* **23** 47
[10] Ziegler J F, Ziegler M D and Biersack J P 2010 *Nucl. Instrum. Methods Phys. Res., Sect. B* **268** 1818–23
[11] Mendenhall M H and Weller R A 2005 *Nucl. Instrum. Methods.* **227** 420–30
[12] Maiorov S A 2009 *Plasma Phys. Rep.* **35** 802–12
[13] White R D, Robson R E and Ness K F 2001 *Comput. Phys. Commun.* **142** 349
[14] Heiche G and Mason E A 1970 *J. Chem. Phys.* **53** 4687
[15] Berd G 1981 *Molecular Gas Dynamics* (Moscow: Mir)
[16] Gott Yu V 1978 *Interaction of Particles with Matter in Plasma Studies* (Moscow: Atomizdat)