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# Modeling of cascade and sub-cascade formation at high PKA energies in irradiated fusion structural materials

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A B S T R A C T

A new theoretical model is developed for the investigations of cascade and sub-cascade formation in fusion structural materials under fast neutron irradiation at high primary knock-on atom energies. Light fusion structural materials: such as Be, C and SiC under 14 MeV neutron irradiation in fusion reactor will have the primary knock-on atoms with the energies up to 1 MeV. It is very difficult to use at such high energies the Monte-Carlo or molecular dynamic simulations [H.L. Heinisch, B.N. Singh, Philos. Mag. A67 (1993) 407; H.L. Heinisch, B.N. Singh, J. Nucl. Mater. 251 (1997) 77]. The developed model is based on the analytical consideration of elastic collisions between displaced moving atoms produced by primary knock-on atoms with some kinetic energies obtained from fast neutrons and crystal lattice atoms. The Thomas–Fermi interaction potential is used here for the description of these elastic atomic collisions. The suggested model takes into account also the electronic losses for moving atoms between elastic collisions. The self-consistent criterion for sub-cascade formation is suggested here which is based on the comparison of mean distance of primary knock-on atoms between consequent collisions of them with the target atoms and a size of sub-cascade produced by moving secondary knock-on atoms produced in such collisions. The analytical relations for the most important characteristics of cascades and sub-cascades are determined including the average number of sub-cascades per one primary knock-on atom in the dependence on its energy, the distance between sub-cascades and the average cascade and sub-cascade sizes. The developed model allows determining the total numbers, distribution functions of cascades and sub-cascades in dependence on their sizes and generation rate of cascades and sub-cascades for the different fusion neutron energy spectra. On the basis of this developed model the numerical calculations for main characteristics of cascades and sub-cascades in different fusion structural materials: Fe, V, C, Al, Be and W are performed here using the neutron fluxes and primary knock-on atom energy spectra for fusion reactors: ITER and DEMO.



## 1. Introduction

In the present paper, we suggest a new self-consistent theoretical model to study sub-cascades formation in irradiated materials. This model is partially based on the results of papers [3,4] and model [5]. This developed model allows calculating the main characteristics of sub-cascades: threshold energy for sub-cascade formation, generation rate of sub-cascades for a given neutron spectrum, average number of sub-cascades per primary knock-on atom (PKA), average distance between sub-cascades, average sub-cascade size. Important efforts have already been carried out to determine the threshold energy $E_{sf}$ for sub-cascade formation [6]. These results are very important for the kinetic consideration of radiation damage (point defects and defect clusters: dislocation loops, voids) accumulation in irradiated materials. Small clusters of radiation defects (dislocation loops, voids) can form into cascades and sub-cascades after relaxation of them during very short time (10–100 ps) [7]. For the further investigations of an evolution of radiation defect structure in the dependence on an irradiation dose we have to know generation rate of defect clusters into cascades and sub-cascades for a given fusion neutron spectrum. All these values can be obtained in the developed theoretical model of this paper.

The main idea of developed theoretical model is based on the comparison of the mean distance $\lambda(E)$ between two successive collisions of a PKA having a kinetic energy $E$ with the average damage zone size $R$ produced by secondary knock-on atoms (SKA) (an average penetration depth of SKA) resulting from the two elastic collisions [5]. The sub-cascades are formed when the following relation is realized $\lambda(E) > R$.

## 2. Developed model for sub-cascade formation and numerical calculations

Most of the previous approaches to calculate $E_{sf}$ [1,5] used the differential cross-sections for elastic collisions, which characterizes

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the probability for a moving atom with the energy $E$ to get an energy $E'$ after an elastic collision. We have to take into account in this model that the SKA can get sometimes a kinetic energy $T$ higher than the residual energy $E'$ of the PKA (and then produces most of the subsequent damage), so these approaches are required to determine the energy distribution function for all moving atoms. In this paper, we develop a new theoretical model for sub-cascade formation in monatomic materials based on our previous paper. [5] Though this model can also be applied for the consideration of sub-cascade formation in multi-atomic irradiated materials using the system of Boltzman kinetic equations [8] for the moving displaced atoms in multi-atomic materials. It takes a separate consideration.

Let us consider the collision between an incident atom with the kinetic energy $E$ and a target atom. We suppose here that $E$ is higher than the displacement threshold energy $\varepsilon_d$ for target atoms ($E >> \varepsilon_d$). After each collision, the incident atom may have the energy higher or lower than the displaced atom. Because both atoms are undistinguished, we will call the incident atom before collision and the atom with the highest energy after elastic collision as the PKA. In the same way, we will call the atom with the lowest energy after the collision as the SKA. These definitions will allow following the fate of the atom with the highest energy for the subsequent atomic collisions. Provided that $E'$ is the highest energy of as-defined PKA after the collision, the two possible configurations are given in Fig. 1.

The cross-section characterizing the type of atomic collisions with the energy transfer higher than $E_{sf}$ has the following form (the ring area in [3], see also [2]):

$$\Sigma(E,E_{sf}) = \int_{E_{sf}}^{(E-\varepsilon_d)/2} dT[\Sigma(E \to E' - T - \varepsilon_d) + \Sigma(E \to T)] = \int_{E_{sf}}^{(E-\varepsilon_d)/2} dTP(E,T)\Sigma(E). \quad (1)$$

The distance $\lambda(E)$ between two successive collisions of the PKAs having a kinetic energy $E$ is given by:

$$\lambda(E) = \frac{1}{N_a \Sigma(E,E_{sf})}. \quad (2)$$

For the elastic differential cross-section, the Thomas–Fermi potential gives the following relation [9,10]:

$$\Sigma(E \to E') = \left(\frac{\pi a^2}{2}\right)\frac{dtpt^{1/6}}{t^{3/2}}\frac{1}{[1+(2pt^{2/3})^{2/3}]^{3/2}}, \quad (3)$$

where $t = E(E-E')/\varepsilon_0{}^2$; $\varepsilon_0 = 2\sqrt{2}e^2Z^{7/3}/0.885a$; $a = 0.53 \times 10^{-10}$ m; $e$ is the electron charge; $Z$ is the charge of the target atom and $p$ is the dimensionless parameter that may slightly vary [11] (here $p = 1.309$).

On the other hand, the average damage zone size (the average penetration depth of SKA) is given by:

$$R(E,E_{sf}) = \int_{E_{sf}}^{(E-\varepsilon_d)/2} P(E,T)R(T)dT, \quad (4)$$

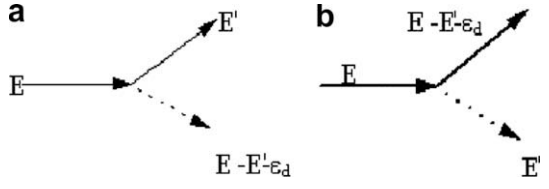


**Fig. 1.** A scheme of an elastic collision according to our definition of PKA and SKA: (a) after collision the incident atom remains as the PKA and has an energy $E'$; (b) after collision the target atom becomes the PKA with an energy $E'$ and the incident atom becomes the SKA.

where $P(E,T)$ is an energy spectrum of SKA normalized to unity. The penetration depth of SKA (sub-cascade size) with an initial kinetic energy $T$ is given by:

$$R(T) = \int_0^T \frac{dT}{(dT/dx)_{tot}}, \quad (5)$$

where $(dT/dx)_{tot} = (dT/dx)_n + (dT/dx)_e$ is the total stopping power for the moving atom including the elastic stopping power $(dT/dx)_n$ and inelastic (electronic losses) stopping power $(dT/dx)_e$ determined from the interpolation scheme of electronic energy loss per each atom from high to low SKA energies as proposed by Biersack and Haggmark [12].

Numerical calculations show that as $E_{sf} \to (E - \varepsilon_d)/2$ (i.e. the highest possible kinetic energy for the SKA) $\lambda(E) \to \infty$ while $R(E,E_{sf})$ keeps a finite value. This means that whatever the energy $E$ of a slowing-down PKA, there is always a value $E_{sf} = E_{sf}(E)$ such as if the SKA energies in two successive collisions are higher than $E_{sf}(E)$, the corresponding damage regions are distinct ($\lambda(E) > R(E,T)$ which means the formation of sub-cascades in elastic collisions is realized).

A set of numerical calculations have been performed to determine the sub-cascade formation energies and the number of sub-cascades $N_{sub}(E)$ induced by a PKA with the initial energy $E$ in the following fusion structural materials: Fe, Cu, V, C, Al, Be and W. The obtained results for $N_{sub}(E)$ are plotted in Fig. 2. It should be remarked that obtained numerical results for the energy dependence of $N_{sub}(E)$ in Cu and Fe (Ni) have a good qualitative and quantitative (20–25%) comparison with the experimental data obtained by Kiritani et al. [6] and the Monte-Carlo modeling results of sub-cascade formations for Cu obtained by Heinisch and Singh [2] and Satoh et al. [3,4].

An important characteristic for the sub-cascade formation is their generation rate: the number of sub-cascades produced per unit time and volume for a given neutron spectrum. This determination requires the knowledge of the cross-section for sub-cascades formation $\sum_{sf}$. Required cross-section was calculated on the basis of elastic neutron scattering using ENDF database for Fe, V, C, Al, Be and W materials. The generation rate of sub-cascades has been determined in listed materials for two neutron spectra (Fig. 3) by the integrating of sub-cascade formation cross-section over given spectrum. These two spectra correspond to neutron energy spectra for fusion reactors: ITER and DEMO. The calculations have been performed by taking into account the elastic collisions for PKAs and

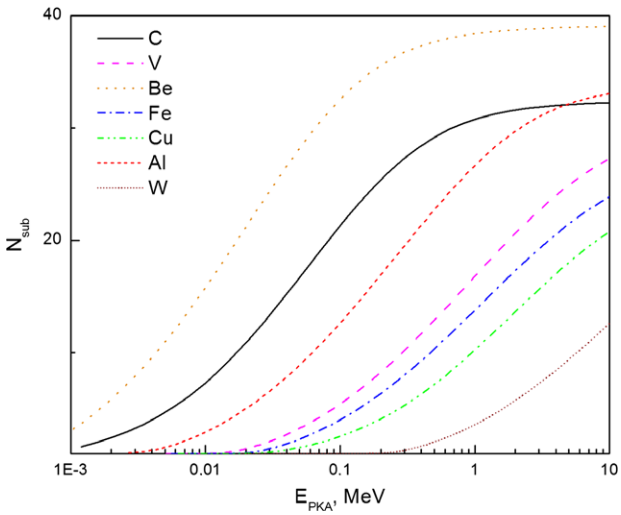


**Fig. 2.** Number of sub-cascades induced by the PKA in Fe, Cu, V, C, Al, Be and W versus PKA initial kinetic energy.

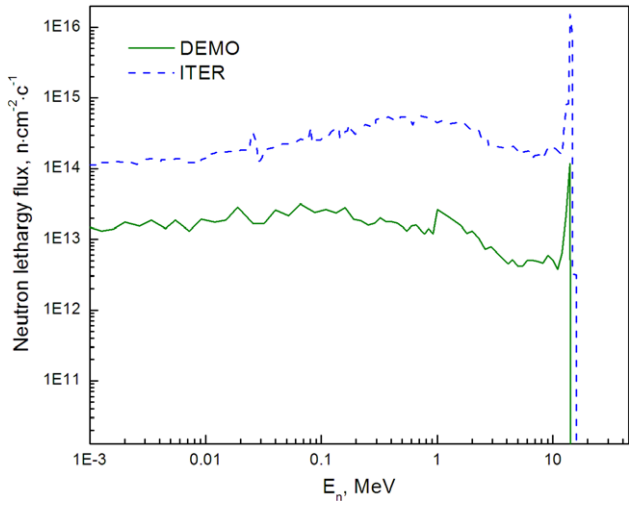


**Fig. 3.** Neutron spectra for fusion reactors: ITER and DEMO.

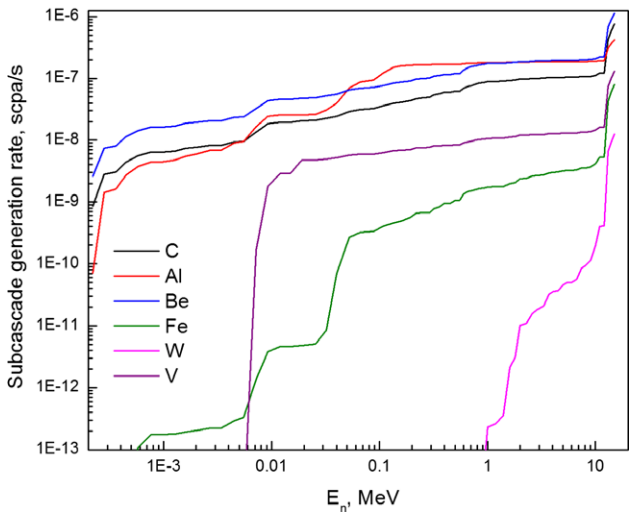


**Fig. 4.** Generation rates of sub-cascades versus neutron energy spectrum for ITER.

SKAs as well as the non-elastic interactions of the SKA with the electronic gas. The results for ITER and DEMO are given in Figs. 4 and 5, respectively. The obtained numerical results in Figs. 4 and 5 show that the generation rates of sub-cascade formation for heavy metallic materials: Fe, V and W for ITER fusion spectrum on the order of value is higher comparing with DEMO. These results correlate with the difference of neutron energy spectra for ITER and DEMO (see Fig. 3). For light materials: C, Al, Be at high neutron energies (higher than 10 keV) this difference has also the one order of value and at low neutron energies (less than 1 keV) this difference stronger (two–three orders of values).

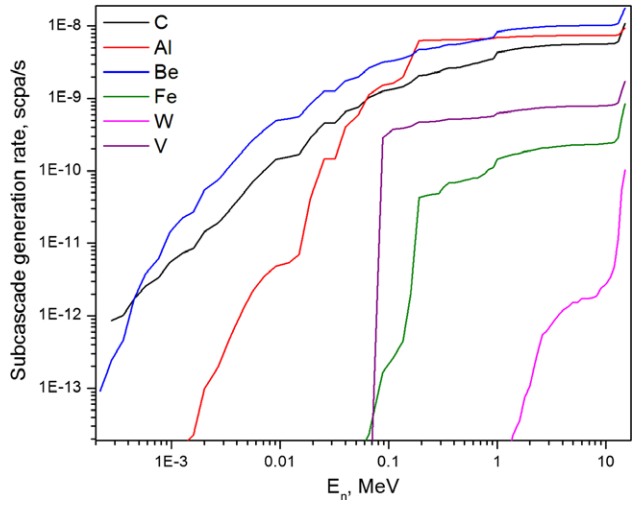


**Fig. 5.** Generation rates of sub-cascades versus neutron energy spectrum for DEMO.

## 3. Conclusion

A self-consistent theoretical model based on the numerical solution of the Boltzmann transport equation in a binary collision approximation has been developed. This approach allows to determine the main characteristics of sub-cascades, such as threshold energy for sub-cascades formation, generation rate of sub-cascades for a given neutron spectrum, average number of sub-cascades per PKA, average distance between sub-cascades, average sub-cascade size. Some of these characteristics were also investigated in different fusion structural materials using the neutron fluxes for fusion reactors: ITER and DEMO. The obtained results for PKA energy dependence of number of sub-cascades correlate with the existed experimental data [6] and the numerical Monte-Carlo modeling results of sub-cascade formation in Cu [3,4]. These results obtained here show that the binary collision model allows to investigating the sub-cascade formation on the collision stage of cascade and give the reasonable results for main important characteristics of sub-cascades as a function of PKA energy.

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