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Monte-Carlo simulations of electrostatic self-charging of tritiated tungsten and beryllium particles

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Abstract. The electrostatic self-charging rate of tokamak dust is investigated using Geant4, a toolkit for the simulation of the passage of particles through matter. To do so, the particles geometrical characteristics, the β disintegration energy spectrum and the deepness of tritium infusion are taken into account. The investigated materials are tungsten and beryllium, the plasma facing components (PFC) of ITER, considered as spherical particles from 20 nm to 200 μm in diameter, both tritiated. Two cases of tritium distribution in the particles are examined. On the one hand, tritium is homogeneously distributed over the whole sphere; on the other hand, tritium is homogeneously distributed within the external 100 nm layer of the sphere. The self-charging rate is assessed through the calculation of the particle exiting electron rate. Based on a tritium inventory of 10 GBq/g, relevant for ITER tokamak environment, our results show that, for a single tungsten or beryllium particle of 10 μm in diameter, the self-charging rate when the tritium is homogeneously distributed within the whole sphere is respectively 2.4 and 1.9 positive elementary charges per second. In the configuration where the tritium absorption is confined in the external 100 nm layer, the charge magnitude raises up to 37.1 and 8.4 respectively.

1. Introduction

Dust particles in tokamak environment affect plasma performance and may be a safety issue in case of incident [1]. Tokamak particles re-suspension is balanced by adhesion forces, mainly electrostatics and Van der Waals interactions [2, 3]. When particles are radioactive, the electrostatic component of the adhesion force needs to be taken into account in order to understand their behaviour. Indeed, due to plasma fuel exposition (especially tritium), dust becomes radioactive and it is well known that radioactive particles exhibit positive self-charging through α and β decay [4, 5]. Usually the self-charging rate for dust particles containing β emitter radionuclides is considered equal to the specific activity of the particles (Bq/particle). Indeed, the considered radionuclides such as ^{137}Cs , ^{132}Te or ^{131}I emit high β energy particles, [6]. Consequently, the electron escape probability from a micron size particle is close to 1. In the case of tritium (^3H) β decay, with the lowest energy β spectrum, further investigations need to be done, especially for dense material like tungsten. The self-charging is investigated using the Geant4 simulation toolkit [7–9] for tungsten and beryllium particles. This kind of



simulations have been done for spatial application with materials charging due to cosmic radiation exposition [10], but has never been realized for radioactive particles self-charging.

This paper presents the results of self-charging rate calculation for single tungsten and beryllium particles, ranging from 20 nm to 200 μm in diameter. For this, the particle geometry and tritium distribution are described precisely in the first part as well as the underlying principle of the β radiation path calculation in matter. The second part focuses on the simulation results which are presented in terms of mean escape probability of electrons from the particle according to diameter. The third part presents the self-charging rate for a given tritium mass specific activity.

2. Particle geometry, tritium distribution and calculation of electron path in particulate matter

The dust particles studied are single spheres with diameters ranging from 20 nm to 200 μm . The simulations are realized for pure tungsten (density = 19,250 kg/m^3) or beryllium (density = 1,850 kg/m^3) particles in vacuum environment. To make a preliminary assessment on the effect of tritium deepness infusion, two limit cases are considered. 1) Tritium is homogeneously distributed in the whole particle; 2) tritium is concentrated in a 100 nm thickness surface layer of the particle. Indeed, case 2 is supported by the fact that, for tungsten and beryllium, the presence of a thin oxide layer would confine the tritium trapping in the first hundred nanometre [2, 11].

The dust particle self-charging due to tritium β decay is computed using the software Geant4 which simulates the radiation pathway through matter using Monte Carlo methods. It computes radiation path through matter, notably for α , β or γ rays, through the interaction probability between the radiation and the matter (atoms), computing the kinetic energy-loss of the radiation at each interaction and the new radiation vector [7]. This software is classically used to assess the efficiency of a radiation detector for various materials and their geometry [8, 9].

To calculate the self-charging due to tritium decay, the path of electrons having the density energy spectrum of tritium is calculated for different dust particle diameters and initial positions of the disintegration inside the particle. As tritium exhibit low energy β decay spectrum (< 20 keV) the calculation of electrons path in matter is realized by the Geant4 set *EM Opt4*, which is a set of electromagnetic physics models disigned for interaction of low energy electrons with matter.

One Geant4 run starts from a random initial position of an electron in the sphere volume (i.e. starting point of the β disintegration), a random initial direction of the electron in the 4π volume. The initial kinetic energy of the electron is chosen according to the tritium β decay energy spectrum. Geant4 then computes transport and energy-loss of this electron in matter. The computation ends when the electron energy vanished, or it escaping from the sphere.

Each Geant4 run corresponds to a define particle diameter (from 0.02 to 200 μm discretised in 1000 size bins) and one millions of electrons, for which initial positions and initial directions are randomly taken in the sphere volume or in the 100 nm external layer. The initial kinetic energy of each electron is chosen to follow the beta decay spectrum that is discretized from 1 to 20 keV in 20 energy bins. Consequently each curve presented in the following section corresponds to a set of $2 \cdot 10^{10}$ calculations of electrons tracking in the particle.

3. Escape probability of electrons

The escape probability of electrons is defined for each particle diameter by the ratio of the electrons that exit the particle by the total number of generated electrons ($20 \cdot 10^6$ for each particle size studied). The energy distribution of electrons is weighted by the tritium β energy distribution.

Figure 1 presents the escape probability of electrons for tungsten and beryllium particles, for the two tritium deepness distribution models (whole sphere and external 100 nm layer).

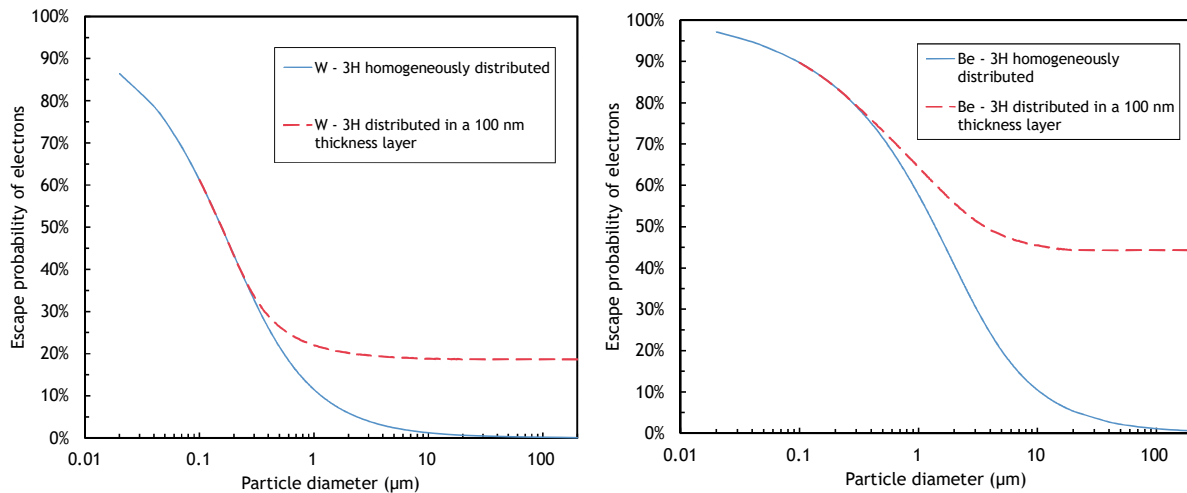


Figure 1 - Escape probability of electrons from W (left) & Be (right) particles, as a function of the particle diameter for the two electron sources distribution

As expected, the two tritium deepness distribution models converge for particle diameter smaller than 200 nm. For larger particle sizes, in the case 1 where the electrons sources are homogeneously distributed throughout the whole sphere, the exiting electrons probability converges toward zero. This means that, the number of exiting electrons becomes negligible compared to the total number of simulated electrons emission. Thus, the larger is the particle, the lesser the exiting electrons probability.

In the case 2, where the electrons sources are only distributed in a 100 nm thickness surface layer, the escape probability converges toward 20 % and 45 % respectively for tungsten and beryllium. This means that, the closer is the distribution source to the surface, the more is the exiting probability. Moreover, the difference between the two limits is due to material density effect on the electron path in matter: the lower density material has the highest limit (the limit should be 50 % for a low density material and a planar surface with infinitesimal thickness: 50 % of electrons will escape from both sides of the surface). Thus, the more is the particle density, the lower the escape probability of electron.

4. Self-charging rate

A tungsten mass activity of 10 GBq/g is selected, as reported from experimental measurements [11]; for comparison, the same mass activity is considered for beryllium particles. The self-charging rate (number of positive charges per unit of time) according to a particle diameter is the product of the escape probability by the isolated particle mass activity (Bq/particle in vacuum).

Figure 2 depicts the self-charging rate for tungsten and beryllium particles, for the two tritium deepness distributions models (whole sphere and surface layer). For each material, the two tritium distributions models converge towards the same values for small particle diameters; this behaviour is due to the similar escape probability of electrons. However, for the largest particle diameters, the self-charging rates increases and diverges between the two tritium distribution models on more than two orders of magnitude. Thus, the closer is the tritium distribution to the particle surface, the higher the self-charging rate. The density effect is perceptible when comparing the tungsten and the beryllium particles. Indeed, for the same mass activity (10 GBq/g), the beryllium (density = 1,850 kg/m³) charging rate is about a decade lower than tungsten (density = 19,250 kg/m³).

For the same particle diameter, the tungsten particle activity is significantly higher than for beryllium because the calculations are based on same tritium mass activity. This explains the counter-intuitive results of higher escape probability of electrons but lower self-charging rate for beryllium and inversely for tungsten.

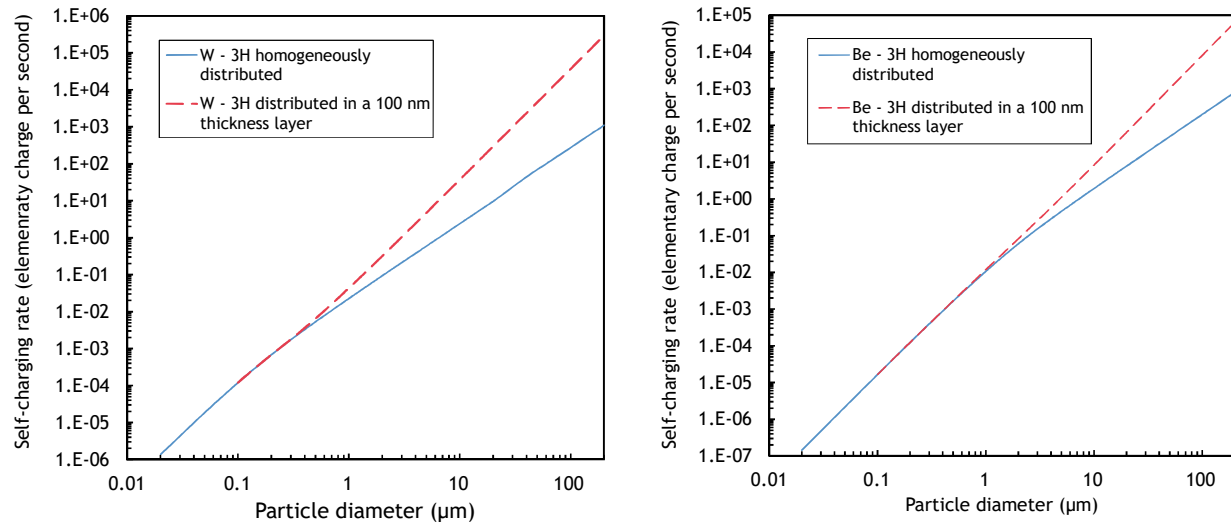


Figure 2 - Self-charging rate of W (left) & Be (right) tritiated particles for the two electron sources distribution

5. Conclusions

The electrostatic self-charging rate of single tungsten and beryllium particles containing tritium is investigated using Geant4. Our results exhibit the dependence of the self-charging rate on three parameters: particle diameter, particle density and tritium deepness distribution.

For the same tritium mass activity, the larger is the particle, the higher the self-charging rate; and the larger is the particle density, the higher the self-charging rate. In the same vein, the closer is the tritium distribution from the particle surface, the higher the self-charging rate.

Considering a realistic tritium inventory of 10 GBq/g, our results reveal that for tungsten and beryllium particles of 10 μm in diameter, the self-charging rate when tritium is homogeneously distributed is 2.4 and 1.9 positive elementary charges per second, respectively. If the tritium is concentrated in a 100 nm surface layer, the self-charging rate for 10 μm particles reaches 37.1 and 8.4 positive elementary charges per second, respectively. Consequently, over a tokamak operation period, the charge accumulation could be high enough to dominate the adhesion force onto the plasma walls. Thus, the presented simulation results on particles self-charging give precious input for more accurate calculations of radioactive dust adhesion force.

Another consequence due to the limited path of the electrons of tritium β disintegration in material is that the tritium inventory carried by airborne particles cannot be measured in real time by conventional continuous radioactive aerosols monitors (CAM's) and a new measurement strategy is needed for atmospheric survey in workplace and exhaust of facility.

Moreover, the results highlight a significant influence of the tritium deepness distribution that is a first step towards the understanding of tritium adsorption profile in dust particles.

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