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Energy loss of 100 keV hydrogen isotopes in materials for nuclear applications

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ABSTRACT

This work studies the energy loss by different mechanisms in materials of nuclear interest (Al, Ti, Fe) when these are irradiated with an hydrogenic beam. The materials chosen were aluminum, titanium and iron, and the selected beam energy was of the order of 100 keV. The mechanisms considered for energy loss are electron excitation and phonon production, for both of them two quantities are defined: one to compare energy deposition by a single ion beam in different materials, the other to characterize several beams impinging a given material.

Introduction

Ion irradiation in metals is a field of great interest due to technological applications such as ion implantation technology, lithography, aerospace and nuclear technology [1–6]. Moreover, the continuum research in condensed matter and in particular metallic materials supports the development of different industries (e.g. steels, aluminum and titanium) [7,8].

Among the physical quantities involved in the interaction of radiation with matter, the range of the particles in the material and the energy dissipation mechanisms must be specifically taken into account. On the one hand, the range is an average distance that characterizes the particle trajectory inside the material until it loses all its energy. On the other hand, the mechanisms for energy loss depend on the characteristics of the material under irradiation and are a function of the beam energy.

Energetic ions interact with matter by three different mechanisms: (1) Collisions with nuclei, (2) Collisions with electrons and (3) Nuclear reactions at very high beam energies. At high non relativistic energies, the ion-nucleus interactions are classical binary collisions under a Coulomb repulsive potential. Since the ion mass is 1800 times higher than the electron mass, the interaction of ions with electrons does not change its trajectory. In addition, nuclear reactions occur at very high incident energies and involve energy loss by the creation of new atomic species from the target atoms. This last phenomena is out of the scope of the present work given the energy range considered.

Due to the large number of collisions that occurs at high energies, each of the three mechanisms are averaged and

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described separately by the corresponding stopping powers [9] leading thus to a total stopping power given by:

$$S(E) = S_e(E) + S_n(E)[+ S_{reactions}(E)] \quad (1)$$

here $S_e(E)$ is the electronic stopping power and accounts for energy losses involving excitation of the electrons present in the target, $S_n(E)$ is the nuclear stopping power that considers the interactions with nuclei in the material, and $S_{reactions}(E)$ stands for the occurrence of nuclear reactions that will be neglected as mentioned previously.

For $S_e(E)$ the excitation processes taken into account are atomic electron and collective (plasmons) excitations, whereas for $S_n(E)$ there are two mechanisms that are considered: the creation of phonons in the material and the radiation damage process. This work studies the energy loss due to phonon production in Aluminum, Titanium and Iron under irradiation of Hydrogen isotopes with energies of the order of 100 keV. As mentioned before these materials are of great importance in several industries and for technological development.

Simulation methods

In order to study the first instants of irradiation in a material, a simple binary collision approximation (BCA) is used. Such a program generates a continually branching sequence of two-atom collisions in each of which a beam atom collides with an initially stationary target atom. The cascade is initiated by the ejection of a primary knock-on atom (PKA) from an atom site by a ion from the beam. This PKA is the first projectile atom in the simulation. It subsequently collides with the first target atom and, in general, both the projectile and target atom emerge from the collision with enough energy to induce a new collision.

To carry out this study the IM3D code [10] (based on BCA) was chosen. It uses the TRIM-SRIM [11] database which has been extensively used to study different situations [12–15]. In addition, it offers the very useful alternative of parallel computing reducing considerably the CPU time.

IM3D [10] is a massively parallel, open-source, 3D Monte Carlo code for simulating the transport of ions and the production of defects within different materials. IM3D can model the 3D distribution of ions and the material evolution associated with the ions energy loss, such as displacement, sputtering, damage, ionization, and phonon production.

The code computes random trajectories of ions to give statistically meaningful data. Each trajectory corresponds to a particle (ion or knocked target atom) with a specified starting position, a given direction, and an incident or primary energy. The particle is tracked as a random sequence of straight free-flight-paths, ending in a binary nuclear collision event where the particle changes its direction of movement and/or loses energy as a result of nuclear and electronic interactions.

The projectile proliferation in a cascade does not continue indefinitely. At each collision, the projectile kinetic energy is subdivided into three contributions: (1) target atom kinetic energy; (2) reduced projectile atom kinetic energy; and (3) electronic excitation energy. As a consequence of this progressive energy subdivision, either one or both collision partners will eventually fail to induce a new collision and, as a consequence, the cascade eventually dies out.

Since the target atoms are in fixed positions at the beginning of each cascade the temperature of the bombarded material is $T = 0$K.W hen the beam particles impinge the target, the temperature will locally rise but this heat will be conducted or radiated out to the surroundings, and the local temperature falls back to 0 K with no more atom movement.

Results and discussion

This section discusses the results of simulations regarding irradiation of Al, Ti and Fe with H and its isotopes. The energy for the proton, deuterium and tritium beams were chosen to be of the order of 100 keV. The energy loss depth distributions for electron excitation as well as phonon production are discussed for selected cases. In addition, data treatment is performed in order to compare materials and characterize different beams.

Fig. 1 shows a comparison of the energy loss depth distributions in aluminum for a 160 keV beam of protons. It is observed that the energy loss due to electron excitations is two orders of magnitude larger than the corresponding due to phonon excitations. In addition, the depth distribution associated with electron excitations is practically almost constant along the entire ion trajectory. On the other hand the depth distribution for phonon excitations reaches a maximum at large depths. This means that the ion loses energy mainly due to interactions with electrons and afterwards it interacts with nuclei producing lattice vibrations. This is verified by comparing this result with Fig. 2 where the range for different ions are exhibited: the position of the maximum of the energy loss to phonon excitation is similar to the range for this energy (160 keV).

However, this behavior for the energy loss depth distributions is understood by looking at Fig. 3 that exhibits the different components of the stopping power for protons in aluminum in the energy range of interest. It is observed that

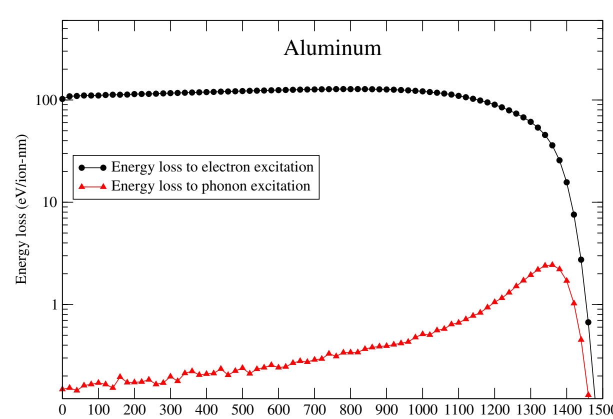

Fig. 1 – Protons energy loss depth distributions to electron (black circles) and phonon (red triangles) excitations in aluminum. Beam energy = 160 keV. (For interpretation of the references to color/colour in this figure legend, the reader is referred to the Web version of this article.)