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PKA energy spectra and primary damage identification in amorphous silica under different neutron energy spectra

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Abstract

Amorphous silica is a key component in windows of heating systems in magnetic fusion reactors and the final focusing of lasers in inertial confinement fusion. Primary knock-on atoms (PKA) energy spectra will be obtained using the SPECTER code for different neutron energy spectra. From those data a systematic analysis of primary damage will be obtained using the TRIM code for high energy recoils, in order to get distribution of cascades and subcascades for these recoil energies to different densities of amorphous silica.

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1. Introduction

This paper describes a computational approach to the quantification of primary damage under irradiation and the effect of neutron energy spectra on the formation of the displacement cascades during a long neutron irradiation of a material such as silica. Amorphous silica is formed by silicon atoms tetrahedrally bonded to oxygen atoms. The initial interaction of a neutron with a lattice atom can lead to the production of high energy recoils, primary knock-on atoms (PKA). The energy transfer reactions between PKAs and other atoms result in a series of displacements which produce non-equilibrium point defects and their clusters, which are fundamental defects present in the primary damage state. Most damage caused by fast neutrons results from the creation of displacement cascades [1]. Processes related to defect formation and migration in materials such as fused silica are very complex, and the results have a very rich variety of defect types and configurations, as well as different charge states and different mobilities.

In the case of inertial confinement fusion reactors [2,3], silica is one of the candidates material for the final optics. In the case of magnetic fusion reactors, silica will be used mostly as windows in diagnostic systems [4,5]. In both cases silica components will need to operate in high temperature and severe radiation environments.

To study radiation damage in this material we have focused our attention on the calculation of

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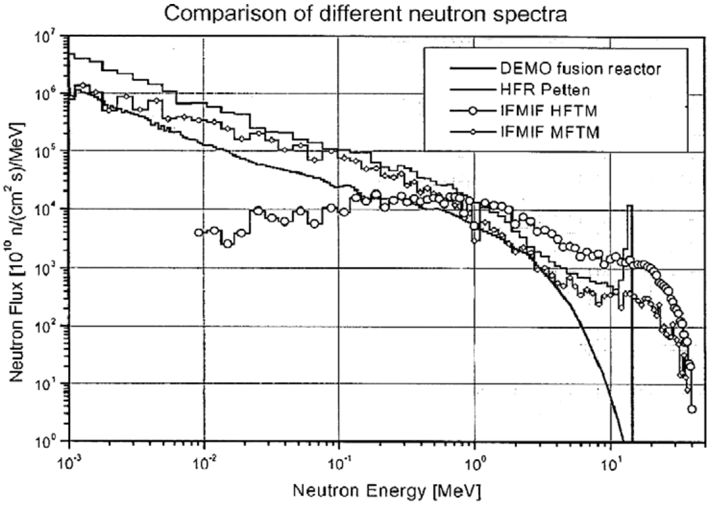

Fig. 1. Neutron flux versus neutron energy for four different systems.

primary knock-on atom spectra under different neutron energy and fluxes for magnetic and inertial fusion energy systems.

2. Methodology: simulation modelling of irradiation of SiO_2

A combined SPECTER [6]/TRIM [7] approach has been used. Neutron radiation damage in materials results from nuclear collision reactions which produce energetic recoil atoms in the host material. These recoiling atoms then generate electronic excitation in the host material (electronic energy loss) and elastic and inelastic collision events (nuclear energy loss). SPECTER deals with the calculation of nuclear energy loss which leads to what is normally is referred to as displacement damage. SPECTER has been employed in this work to obtain the primary knock-on atom distributions for silicon and oxygen in the silica.

On the other hand, TRIM is a Monte Carlo computer program based on a universal potential. It calculates both the final 3D distribution of the ions and also all kinetic phenomena associated with the ion's energy loss: target damage, sputtering, ionization, and phonon production. TRIM has been used to obtain the recoil energy distributions derived from both silicon and oxygen ion beams on silica material from which the cascade database is constructed.

We have considered in this study neutron sources with different energy spectra, including some facilities that are in use such as the HFR-Petten (High Flux Reactor) or planned such as the IFMIF (International Fusion Materials Irradiation Facility) MFTM (Medium Flux Test Module) and HFTM (High Flux Test Module). These spectra are shown in Fig. 1 together with that of a fusion DEMO reactor. It can be noted, in this figure, that neutron energy ranges for each spectrum are different. In order to consider in our calculations using SPECTER code the same neutron energy ranges for all neutron spectra, we have established a lower energy threshold at a neutron energy of 10^{-2} MeV and we have neglected neutrons with energy greater than 14 MeV. In this way, the neutron fluxes considered in our simulations are a fraction of the actual total neutron flux for each facility. These fraction are shown in Table 1.

In addition, we have carried out calculations for a 14 MeV neutron energy spectrum with a neutron flux of 9.36×10^{15} n cm^{-2} s^{-1}. In all the cases the irradiation period was one year.

Integral recoil spectra obtained by SPECTER are shown in Fig. 2 for silicon and oxygen ions, for the different neutron energy spectra and fluxes mentioned above. It can be noted that the shape

Table 1
Main characteristics of neutron fluxes under consideration

Fusion concept	Neutron flux between 10^{-2} MeV and 14 MeV (n cm^{-2} s^{-1})
DEMO	2.26×10^{15} (≈93.77% of total flux)
HFR	2.26×10^{14} (≈87.6% of total flux)
IFMIF HFTM	7.02×10^{14} (≈92.73% of total flux)
IFMIF MFTM	5.58×10^{14} (≈90.58% of total flux)

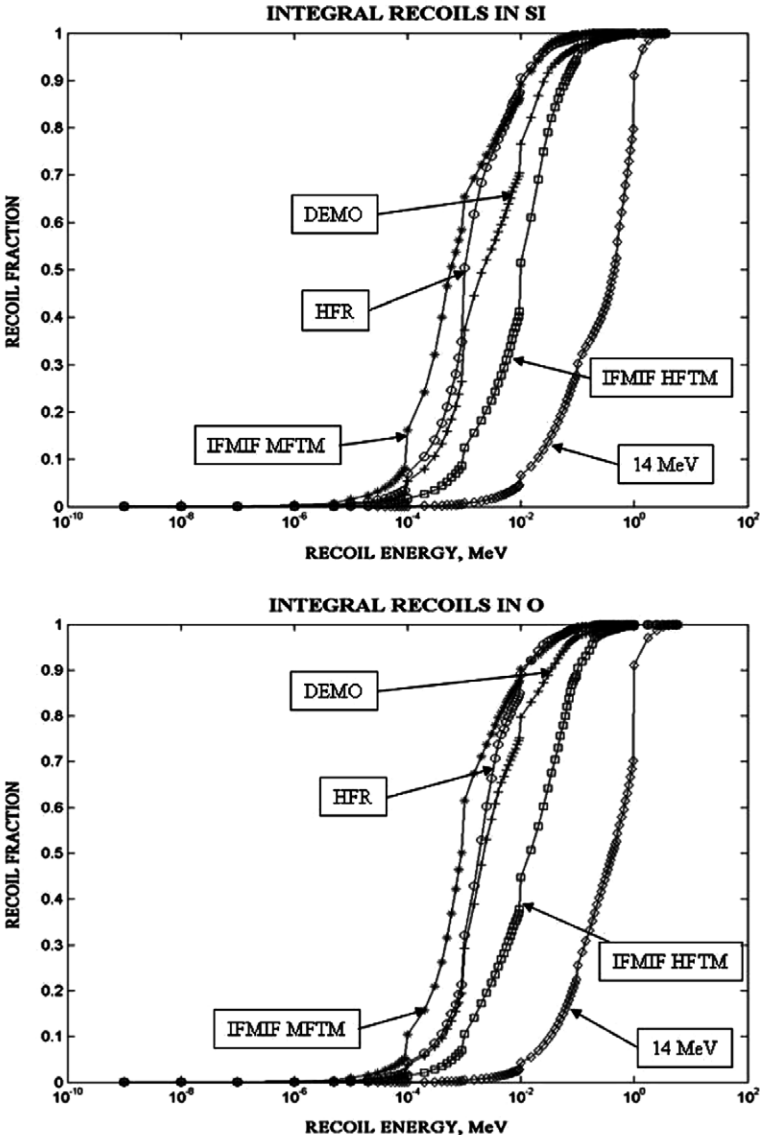

Fig. 2. Integral primary recoil spectra versus energy for silicon and oxygen ions under different neutron energy spectra.

of all the curves is very similar with exception of that corresponding to 14 MeV neutrons. In this case, a shift towards higher kinetic energy of the primary recoil spectrum can be observed. It can be considered that all primary recoil energies are lower than 100 keV except for the case of 14 MeV neutron spectrum.

Taking into account the SPECTER results, we have chosen the PKA energy of 100 keV for subsequent calculations because it is nearly the maximum value for all the spectra except the 14 MeV source (>90% of PKA are below 100 keV). PKA at or below this energy will account for most of the damage production in the material during the operation of fusion energy systems. The original 100 keV PKA will lead to the formation of many lower energy cascades by collisions with other atoms in the material.

The second part of our study is focused on obtaining the main characteristics of the primary damage pattern produced in amorphous silica for oxygen and silicon recoils with a 100 keV energy. To get the distribution of cascades and subcascades for this recoil energy, we have employed the TRIM code with a 500 nm thick slab of silica at different densities in order to take into account the density distribution that characterizes amorphous silica.

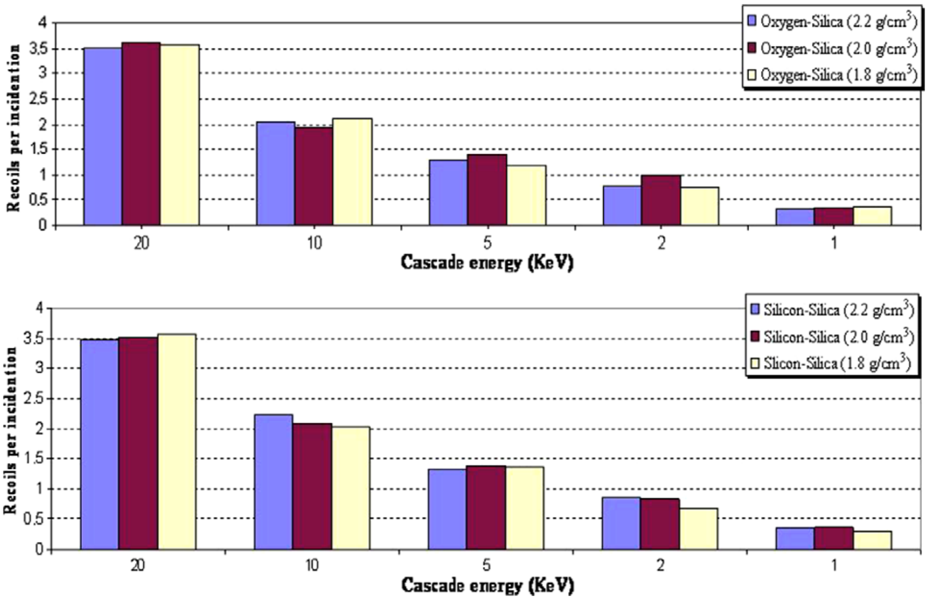

Fig. 3. PKA energy spectrum decomposition per 100 keV incident ion, for oxygen and silicon in silica material.

Some studies [8] show that the density of amorphous silica presents a range of values between 1.4 and 2.8 g cm^{-3}. The density values considered have been 1.8, 2.0 and 2.2 g cm^{-3}.

To obtain statistically significant results, averages of 100 ions were obtained for each case, as shown in Fig. 3. The data extracted from each run, after being appropriately sorted, provides the necessary information for identifying the main characteristics of the primary damage pattern.

3. Conclusions

The results indicate that for the silica densities considered in this work, most of the displacement damage is due to displacement cascades with recoil energies of 20 keV. For silicon recoils, Fig. 3 shows that when density increases, the fraction of 20 keV energy recoils decreases. However, this variation is not observed for oxygen recoils.

On the other hand, we also conclude that the total number of 20 keV recoils per 100 keV incident ion is similar for both cases oxygen and silicon recoils. It can be noted that with slight variation, in the case of silicon, the number of recoils increases with density at energies of 10, 2 and 1 keV. In the case of oxygen, a different behaviour is observed than for the case of silicon.

Currently we are starting a collaboration with Centro de Investigaciones Energética MedioAmbiental y Tecnológica (CIEMAT) and Universidad Autónoma de Madrid with the goal to compare our results with experimental data, using accelerated ions incident on silica samples.

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