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Insight into the materials choice for inertial fusion energy reactors considering radiation damage: Neutron irradiation intensities and basic knowledge from multiscale modeling

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Abstract

A review of structural materials choices under irradiation in fusion environments is presented. Results on the neutron source term and the intensities in the structural materials as a function of pulse time, energy, and protection is given. The role of multiscale modeling for understanding the basic physics in irradiated materials is explained, and simulations of metals under pulse irradiation and SiC are reported.

Keywords: Inertial fusion; Multiscale modeling; Neutron irradiation; Pulsed damage; SiC; Target emission

1. INTRODUCTION

It has been extensively remarked in the research into heavy inertial fusion (HIF) energy that the selection of appropriate materials will certainly be one of the key issues in its development. The radiation environment (neutron, photons, charged particles) in which the materials are working is one of the basic problems. The effect of irradiation can change the expected responses from the materials. Inertial fusion technology offers some *nonmaterials* solutions for such problems considering the availability of blanket protections (gas, liquid/thick, film) of the structural materials in the blanket and bulk structure. However, that is only one part of the solution; the other is dependent on the right selection of the material. The present choices of structural materials are based both on low activation and resistance to irradiation; ferritic-martensitic alloys, SiC as base of composites, and vanadium alloys are the present proposals. The input parameters for the evaluation of radiation damage is the time and energy neutron flux distribution into the materials, which is described below for two different blanket protections. The intrinsic characteristic of HIF leads to pulsed radiation damage, and the present knowledge in this area from using multiscale modeling (MM) is presented, showing the few accumulated results to present a clear picture of the problem. In addition to the accumulated micro- and macroscopic experimental results under the magnetic fusion program, and their supporting theories (if any), the MM approach is reaching important results in understanding the final modification of the materials responses under irradiation from basic principles. A key justification for MM is its predictive character, which allows not only new understanding of the link from basic to final mechanisms, but reliable extrapolation from experiments. We are presenting results using MM on SiC and pulsed irradiation of Fe. The support of MM conclusions by experimental programs (VENUS-II, REVE) is actually a key aspect (Perlado *et al.*, 2002*a*).

2. MATERIALS IN THE FUSION PROGRAM

In both options, magnetic and inertial fusion, the structural materials will be chosen in connection with the blanket design that also can work as an efficient protective wall in the case of inertial fusion reactors. Two main options actually represent the lines of reactor systems in IFE: HYLIFE-II (Moir, 1995), OSIRIS and SOMBRERO (Meier *et al.*, 1992),

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together with the work developed by the ARIES team (Raffray *et al.*, 2002) to arrive at conclusions about the specific components of such reactors. Blankets in magnetic reactors are a combination of breeder, coolant, and specific structural materials that include He or water-cooled ceramic breeder, self-cooled Li, LiPb, Flibe blankets, and ferritic, vanadium, and composites structural materials (Kleykamp *et al*., 2002).

Reduced-activation ferritic/martensitic steels are the first option from the point of view of applicability: F82H (7.5 Cr-2WVTa), JLF-1 (9Cr-2WVTa), EUROFER 97, and additional 7-9 Cr classes of steels. The effect of He, generated by transmutation in fusion environments and producing severe embrittlement and swelling in these steels, is the main question for final consideration. However, recent results (experiments up to 80 appm by using B-10 and molecular dynamics simulations) even at 600 appm He concentration show no enhanced embrittlement and hardening. It seems that in ion implantation by Ni experiments the dominant effect came from the Ni itself, the reason for that good resistance being the high capacity for trapping of He atoms by dislocations, grain boundaries, and carbide/matrix interfaces (Kimura *et al.*, 2002). Another limitation of these steels is the allowed temperature (≈600°C) which guide to the research on the Oxide Dispersion Steels (ODS). The essence of ODS is the inclusion of Y_2O_3 particles (with concentrations 0.3 to 0.5 wt%) in the nanoscale range (2–3 nm diameter) which act as strong sinks for defects generated by irradiation at the particle–matrix interfaces. Specifically, they pin dislocation and they are not dissolved at high temperatures, not arriving at recrystalization up to 1373 K. A gain in yield strength of 50% is demonstrated which is maintained for high temperatures. The advantages in creep up to 700°C and cycle fatigue with respect to the conventional reduced-activation steels are also proved. The problem still remains the production techniques. Concerning SiC and composites from it, their radiation stability is dominated by the differential swelling between the SiC fiber that are not fully dense or crystalline, carbon interphases, and β SiC matrix. An increase in the deep/basic understanding of the damage mechanisms in this material is vitally necessary to complement the data bank emerging from experimental results in the fusion programs. Concerning vanadium alloys, the main candidate is V-4Cr-4Ti, and a full description of impurity redistribution and precipitation, deformation, and irradiation effects is in progress.

3. NEUTRON SOURCE AND FLUX IN THE STRUCTURAL WALLS

The first parameter to know when studying neutron damage in IFE chambers and structures is the neutron intensity and its dependence on time and energy. No specific references are given for these parameters in the designs and a short summary of new evaluations performed at DENIM is here presented. A systematic analysis has been done which includes: (1) different compression of the target when ignited and burning (constant density, two different densities that correspond to spark and surrounding zones, and one uniform density including C layer), (2) different types of protection (LiPb, Flibe), and (3) thickness of protection (60 and 100 cm) as the main variables.

We show here results for time dependence of neutron flux in the Fe layer that represents the most internal structural layer. The liquid main protection is assumed to be at 4 m radius of the center of the chamber (target position) with a baseline thickness of 60 cm. After the protection, the structural materials (Fe) is included (10 cm thickness).

The results show a very different characteristic for both protections (Fig. 1). The neutron source has an intensity of 2×10^{20} n/pulse. In the case of LiPb, the maximum is attained 0.2 μs after a slow increase in the intensity, which is not observed in the case of Flibe. For Flibe the maximum is obtained at the first arrival of neutrons in the layer after 0.1 μs (Fig. 1). The neutron spectra are also different (Fig. 2). In the case of LiPb, a second maximum is observed at 1 μs. We explain these differences for two reasons: (1) the densities of Flibe (2 $g \cdot cm^{-3}$) and LiPb (9.51 $g \cdot cm^{-3}$) are very much different, (2) the $(n, 2n)$ and $(n, 3n)$ are very important nuclear reactions with Pb which strongly moderate the neutron spectrum emerging from the protection with a clear delay in the time of arrival.

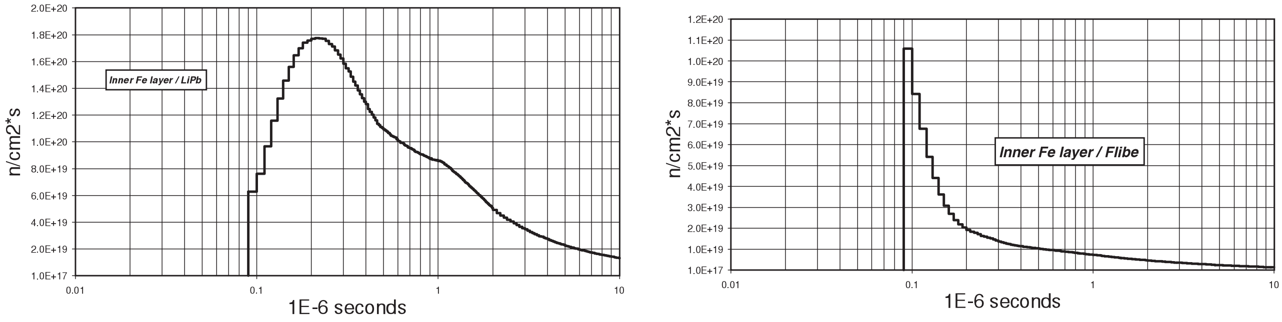

Fig. 1. Flux ($n \cdot cm^2 \cdot s^{-1}$) in Fe inner layer versus time after the source emission (microseconds) for LiPB protection (left) and Flibe protection (right) with 60 cm thickness.

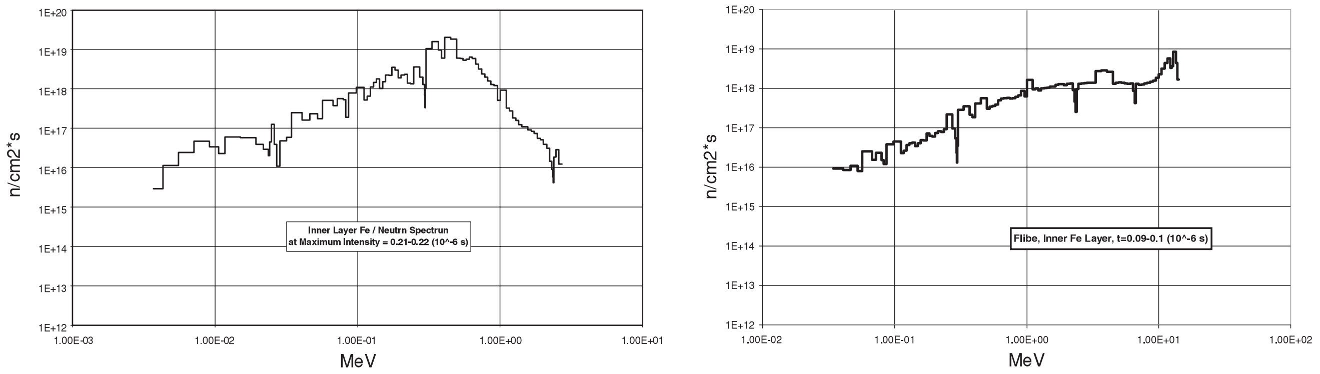

Fig. 2. Neutron spectra at times of maximum intensity for Fe inner layer in the case of LiPb (left, 0.2 μs) and Flibe (right, 0.1 μs) protections.

4. MULTISCALE MODELING OF RADIATION DAMAGE TO MATERIALS

One of the most powerful tools for radiation damage studies actually is multiscale modeling, which is traced in all its steps in Figure 3. This is, with restrictions because of the reliability of the parameters used in the different levels of description, a unique tool to have predictive capability based on physics inside. The main goal is to follow the real mechanisms involved in the radiation damage from the entering of the neutron in the lattice up to the change in the macroscopic properties requested to the material (conductivity, mechanical integrity, etc.).

Nuclear data for neutron reaction and kinematics giving the primary knock-on atom distribution, cascades quantification, and emerging freely migrating defects, diffusion of defects in the lattice with their clustering and dissociation, and the final interaction of those defects with the dislocation in the crystal modifying the mechanical responses describe the full modeling. Present results from molecular dynamics give good insights into physics mechanisms that cannot be observed in experiments. Connection with microscopic observation is actually performed by kinetic Monte Carlo, and defect structures and energetics are becoming progressively well known (Marian *et al.*, 2002). First comparisons with microstructure have been recently given (Almeida *et al.*, 1999; Diaz de la Rubia *et al.*, 1999; Perlado *et al.*, 1999; Soneda *et al.*, 1999; Caturla *et al.*, 2000; Wirth, 2001) and specific national and international programs are being conducted (VENUS Spanish, REVE International); the situation is similar to that of the nuclear data buildup sometime ago in reactors physics. The connection with the macroscopic has very scarcely been done but the basis for it has been established (Diaz de la Rubia *et al.*, 2000).

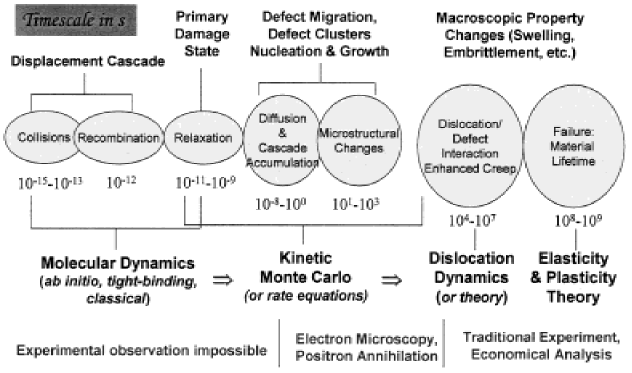

Fig. 3. Scheme of multiscale modeling from the atom cell to the macroscopic.

5. RESULTS ON RADIATION DAMAGE USING MULTISCALE MODELING SIGNIFICANT FOR INERTIAL FUSION

Among the different results obtained by DENIM in the recent past, we note two: pulsed irradiation simulation of a sample of Fe by a time dependent flux (Perlado *et al.*, 2002*b*); and the systematic research on the radiation damage physics in SiC, which includes the development of quasi *ab initio* calculations for obtaining the key parameters for correcting defect diffusion (Perlado *et al.*, 2002*c*). In pulsed irradiation, we consider dose rate (0.1–0.01 dpa/s), the pulse frequency (1–10 Hz) and the temperature (300–600 K). Each object in the simulation box has an associated set of probabilities corresponding to the potential events. All simulations have been conducted in a 300-nm cubical box. The results which represent the microstructure are given in terms of cluster size and concentration, and they have been obtained with the accumulation of 500 pulses in the "high" dose rate case and of 5000 in the "low" dose rate case, which gives a total dose of 1×10^{-4} dpa. From the comparison between the pulsed and continuous irradiation, we conclude at this low dose that the cluster accumulation was essentially similar when the average dose rate were similar (Fig. 4).

We developed a tight binding molecular dynamics scheme (TBMD) with which we can simulate a perfect crystal of β-SiC and its evolution in time. We can manage a different quantity of atoms in the crystal simulation box, with a max-

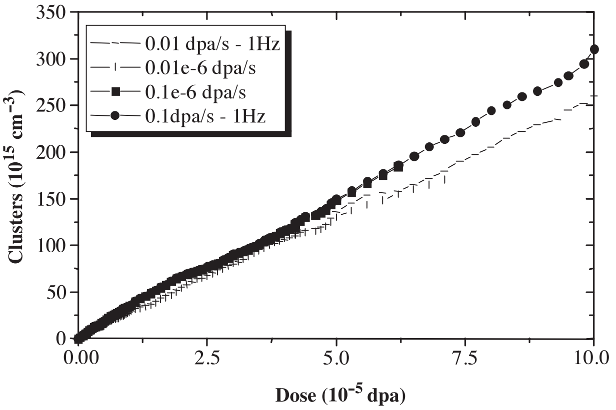

Fig. 4. Cluster density (10^{15} cm^{-3}) versus dose in 10^{-5} dpa.

imum quantity established of 1000 atoms. The pair correlation function $g(r)$ (Fig. 5) indicates the probability of finding an atom of a different species in the nearest neighbor distance of the diamond configuration of β-SiC. To obtain this result we have used a canonical simulation with 216 atoms in the simulation box at 600 K and 7000 time steps. We can appreciate that the material is not amorphous; consequently, the crystalline structure is maintained, allowing us to study the different geometries of the defects that we are able to install. Besides, we can also study separately the pure silicon as well as the pure carbon. In a microcanonical simulation, the energy should be maintained at a constant; thus we will be able to confirm with certainty that in each iteration, the equations of the repulsive term, the diagonalization into the Hamiltonian of the matrix elements, and the Helmann–Feynman theorem contribute in a consistent way, and reproduce efficiently the physics that exists in a β-SiC crystal exposed to that temperature. By using microcanonical simulation density, volume, energy (NVE), with sufficient time steps, a perfect conservation of the energy has been observed in dynamical simulation, which gives us confidence in the determination of the defects energetic for SiC.

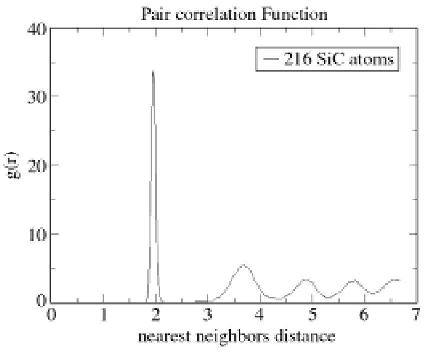

Fig. 5. Pair correlation for SiC.

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