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Activation and damage of fusion materials and tritium effects in inertial fusion reactors: Strategy for adequate irradiation*

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Abstract

Long term research in low activation materials is being pursued in fusion programs and the assessment of allowable elements and/or impurities from safety and repository reasons are being studied at Instituto Fusión Nuclear (DENIM), using ACAB code, for national ignition facility (NIF) and inertial fusion energy (IFE) reactors. Uncertainties in nuclear data are being considered, and experiments for validation of modeling will be presented. Multiscale simulation of radiation damage is now starting to be compared with experiments, and results on the simplest material can be reported as a function of impurities, temperature, and dose. Molecular dynamics (MD) allows us to identify stress-strain curve of FeCr ferritic steels under irradiation, and macroscopic conclusions can be advanced using simple models. However, a neutron source of enough intensity and adequate energy spectrum is needed which will be very peculiar in the case of pulsed IFE, as we claimed in past years. Development of international fusion materials irradiation facility (IFMIF) will be commented and compared with solutions such as spallation, and others using ultra-intense lasers for obtaining required irradiation magnitudes. Research on radiation damage in SiC composite is being pursued at macroscopic level, but basic knowledge is scarce. A systematic identification of type of stable defects is being presented with a new tight binding MD technique. Our research on simulation of silica irradiation damage will also be presented. The role of tritium, when elemental tritium (HT) and titrated water (HTO) derive in organically bound tritium (OBT) will be explained. The deposition and absorption processes are now being considered in our calculations giving more precision and accuracy to our conclusions of dosimetry effects. The role of HT versus HTO and the importance of re-emission process will be remarked, together with the long-term role of OBT.

Keywords: Activation; Inertial Fusion; Radiation Damage; Tritium

1. ACTIVATION OF MATERIALS: SAFETY AND ENVIRONMENTAL ISSUES

The physics of fusion and especially inertial fusion energy related topics have experienced significant progress in recent years (Canaud *et al.*, 2004; Deutsch, 2004). However, in order to turn inertial confinement fusion into an energy source that is economical and acceptable to the public, some major technological problems remain to be solved. These problems are the availability of cheap and reliable fusion targets (see chapter by E. Koresheva, D. Goodin, and T. Norimatsu in Mank *et al.*, 2005; Borisenko *et al.*, 2003), the problem of adequate materials resistant to very intense and pulsed irradiation, and that of activated material from an inertial fusion power plant (Perlado & Sanz, 1993). The activation problem as well as the associated tritium problem is the focus of discussion for many years at very different reactor concepts (Velarde & Perlado, 2002; Tahir & Hoffmann, 1997; Perlado & Sanz, 1993; Beller *et al.*, 1993). Also,

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heavy ion drivers have to deal with activation problems due to beam losses (Mustafin *et al*., 2002; Fertman *et al*., 2002). Certainly activation was extensively used as a good and efficient diagnosis of core performance in target implosion (Azechi *et al*., 1991*a*, 1991*b*), and appear in the routine activities of experimental inertial confinement facilities (Manes *et al*., 1985; Andre *et al*., 1994).

In the field of computational modeling for safety and environmental (S&E) analysis, our main contribution refers to the computational system ACAB (Sanz, 2000) that is able to compute the inventory evolution as well as a number of related inventory response functions useful for safety and waste management assessments. The ACAB system was used by the Lawrence Livermore National Laboratory (LLNL) for the activation calculation of the NIF design (Sanz *et al*., 2003) as well as for most of the activation calculations, S&E studies of the HYLIFE-II and Sombrero IFE power plants with severe experimental testing at rotating target neutron source (RTNS-II) at the University of Berkeley (Latkowski *et al*., 2003), see Figure 1. Pulsed activation regimes can be modeled (key in inertial confinement fusion devices test/experimental facilities and power plants), and uncertainties are computed on activation calculations due to cross section uncertainties. In establishing an updated methodology for IFE safety analysis, we also introduced time heat transfer and thermal-hydraulics calculations to obtain better estimates of radionuclide release fractions. Off-site doses and health effects are dealt with by using MACSS2 and developing an appropriate methodology to generate dose conversion factor (DCF) for a number of significant radionuclides unable to be dealt with the current MACSS2 system. We performed loss of coolant (LOCA) and loss of flow (LOFA) analyses for the HYLIFE-II design. It was demonstrated the inherent radiological safety of HYLIFE-II design relative to the use of flibe. Assuming typical weather conditions, total off-site doses would result below the 10-mSv limit. The dominant dose comes from the tritium in HTO form. In the Sombrero design, a severe accident consisting of a total LOFA with simultaneous LOVA was analyzed. Key safety issues are the tritium retention in the C/C composite, and the oxidation of graphite with air that should be prevented. The activation products from the Xe gas in the chamber are the most contributing source to the final dose leading to 47 mSv. We also analyzed the radiological consequences and the chemical toxicity effects of accidental releases associated to the use of Hg, Pb, and Be, as IFE materials under HYLIFE-II framework scenario. For those three materials, the chemical safety requirements dominate strongly over radiological considerations. Also, the role of clearance as waste management option for HYLIFE-II was explored. For the confinement building, which dominates the total volume of the waste stream, all the material could be released from regulatory control for unconditional re-use after about one year of cooling following plant-shutdown. We also explored liquid wall options for tritium-lean fast ignition IFE power plants. Many single, binary, and ternary molten-salts were evaluated for their S&E characteristics, as well as for the required pumping power. In analyzing the impact of cross section uncertainties on the contact dose rate from the activated concrete-unite outer shell of the NIF reaction chamber, it is shown that current cross sections allows a reasonably confidence in the results. Regarding IFE, uncertainties in the prediction of the neutron induced long-lived activity in all the natural elements shown that for the HYLIFE vessel a significant error is estimated in the activation of several elements, while the estimated errors in the Sombrero case are much less important.

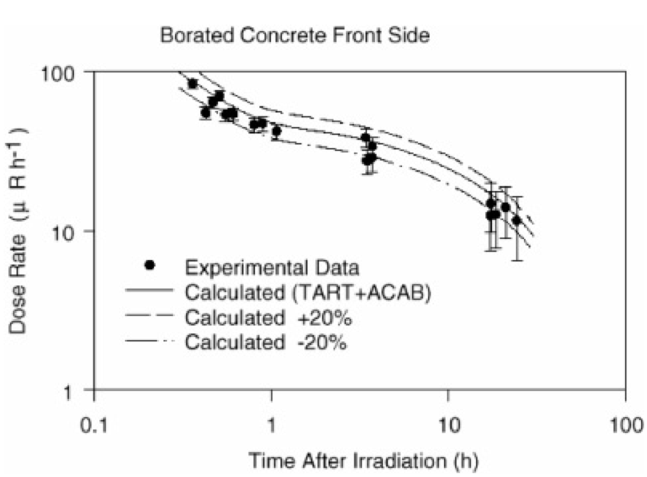

Fig. 1. Contact Dose for Borated Concrete in front of detector in the back side of the bloc. Validation of TART-ACAB code versus experiments in RTNS-II neutron source.

2. RADIATION DAMAGE OF FUSION MATERIALS

Ferritic-martensitic steels (in their more advanced type using experimentally testing oxide dispersion strength (ODS) technique), composites based in SiC, and vanadium alloys are those materials presently under discussion as structural materials, together with C, Be, and W, as first wall materials, and some ceramics (silica, alumina, . . .) as optics and insulators elements. A systematic experimental program is partially pursued in different countries to assess their performance under the specific conditions they will be working on. It is very certain that a large and new irradiation facility is critically needed, and international fusion materials irradiation facility (IFMIF) will cover such role. At present, multiscale modeling (MM) is getting a large role in obtaining predictive characteristic and defining the needed experiments. A common methodology work appears for fusion programs but also for other nuclear systems such as fission (advanced fission reactors/generation IV and accelerator driven systems for transmutation) with coincidences in some of the analyzed materials. Key value has the validation of MM against specific experiments step by step at the microscopic and macroscopic levels and real understanding of damage processes, and effects of alloying and impurities elements. Microscopic parameters (using MD and DENIM

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models), which identify the effect of irradiation through new defects formation and diffusion, are being generated for some specific metallic materials (Fe, binary alloys FeCr, FeCu, V. . .) and their diffusion conducted by Monte Carlo (Perlado *et al*., 2004). Next step is being their interaction with dislocations (dislocation dynamics) and study of nucleation in the presence of He. That effect of He in FeCr alloys is certainly critical. We also derive macroscopic magnitudes using small-scale MM models in short simulation times by using MD defect-dislocation studies under stress (Marian *et al*., 2003). We modeled pulse radiation damage, and we progress in the microscopic validation of MM with experiments using pure and ultra-high pure Fe (effect of impurities) through a national simulation-experimental program using ions irradiation (Perlado *et al*., 2004). Our work is also concentrated on two IFE key materials (SiO_2/optics, SiC/low activation advance material). A MD "tight binding" scheme was fully developed for β-SiC to understand the microscopic phenomena of the native defects and its diffusion at different temperatures. We reach an extraordinary good agreement among our calculated defects energetic and those results obtained using sophisticated and expensive method such as *ab-initio* at 2000 K. We observe that β-SiC crystal remains perfect with its typical cubic structure at that temperature, and we have shown that the carbon atoms do not diffuse into the crystal. Self-interstitial silicon atom prefers the relation with atoms of the same specie due to the effect that the repulsive force of the silicon atoms is larger than the repulsive forces of the carbon atoms (Salvador *et al*., 2004). MD is also being used to study the defects produced in fused silica by energetic atoms, neutron and gamma irradiation. We determine the structure factor, the bond angle distribution, coordination and ring statistics, and we conclude very good agreement with measurement of generation of fused silica glass (Mota *et al*., 2004), see Figure 2. Threshold displacement energies was computed as a function of the direction of movement of PKA, and cascades of 5 keV are being actually extended to 10 keV. Two modeling-experimental programs were started in 2004 with CIEMAT for Silica analysis, which will be extended in the future to Alumina and other materials of first wall and ceramics insulators.

3. TRITIUM ATMOSPHERIC DIFFUSION AND ENVIRONMENTAL PATHWAYS TO HUMAN CHAIN

A large and completely new work was performed in the analysis of consequences of tritium release according with expected source emission from IFE conceptual reactors and others nuclear systems (Velarde *et al*., 2004). Key aspect here is to consider all chemical forms of tritium (HT and HTO) and their conversion to organically bound tritium (OBT) with soil processes and consequences of re-emission to atmosphere; see Figure 3. We report several important conclusions for the primary and, namely, secondary phases

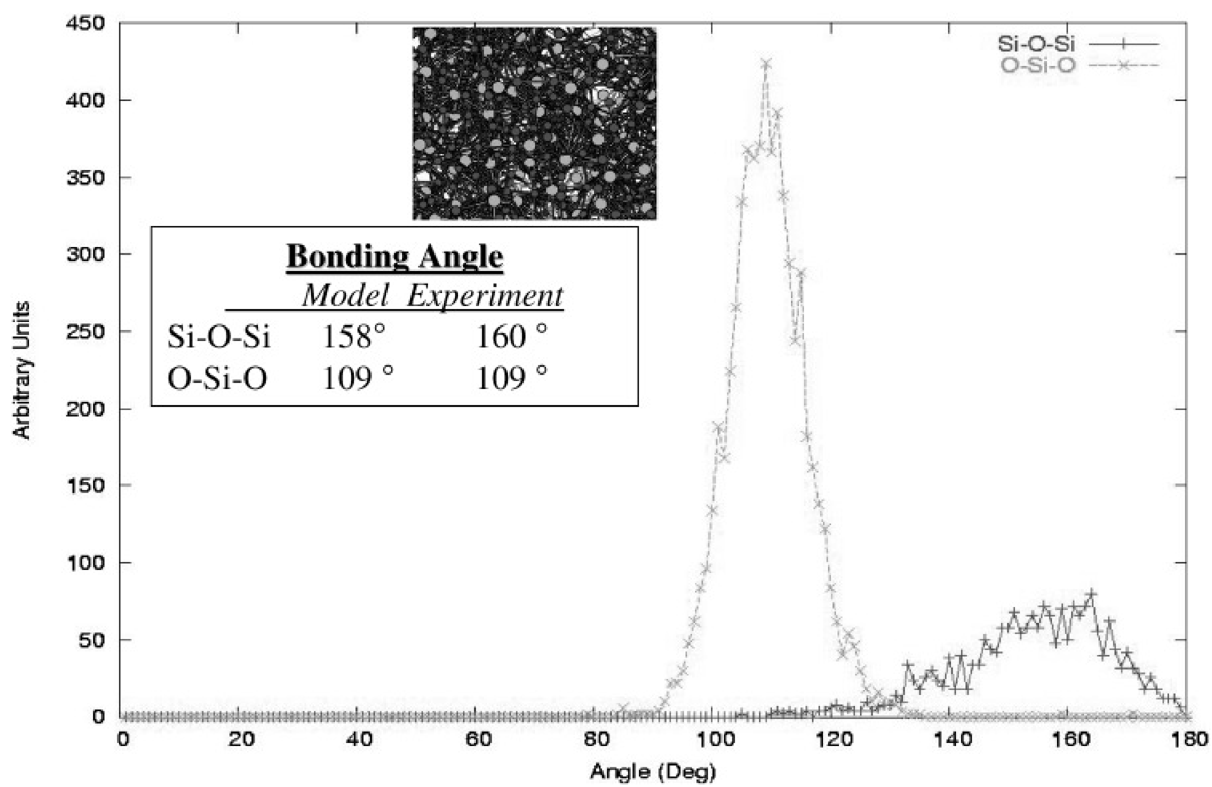

Fig. 2. Generating Amorphous Glass Silica for Threshold Displacement energy study and irradiation experiments with cyclotron radiation (CIEMAT). Validation versus experiments.

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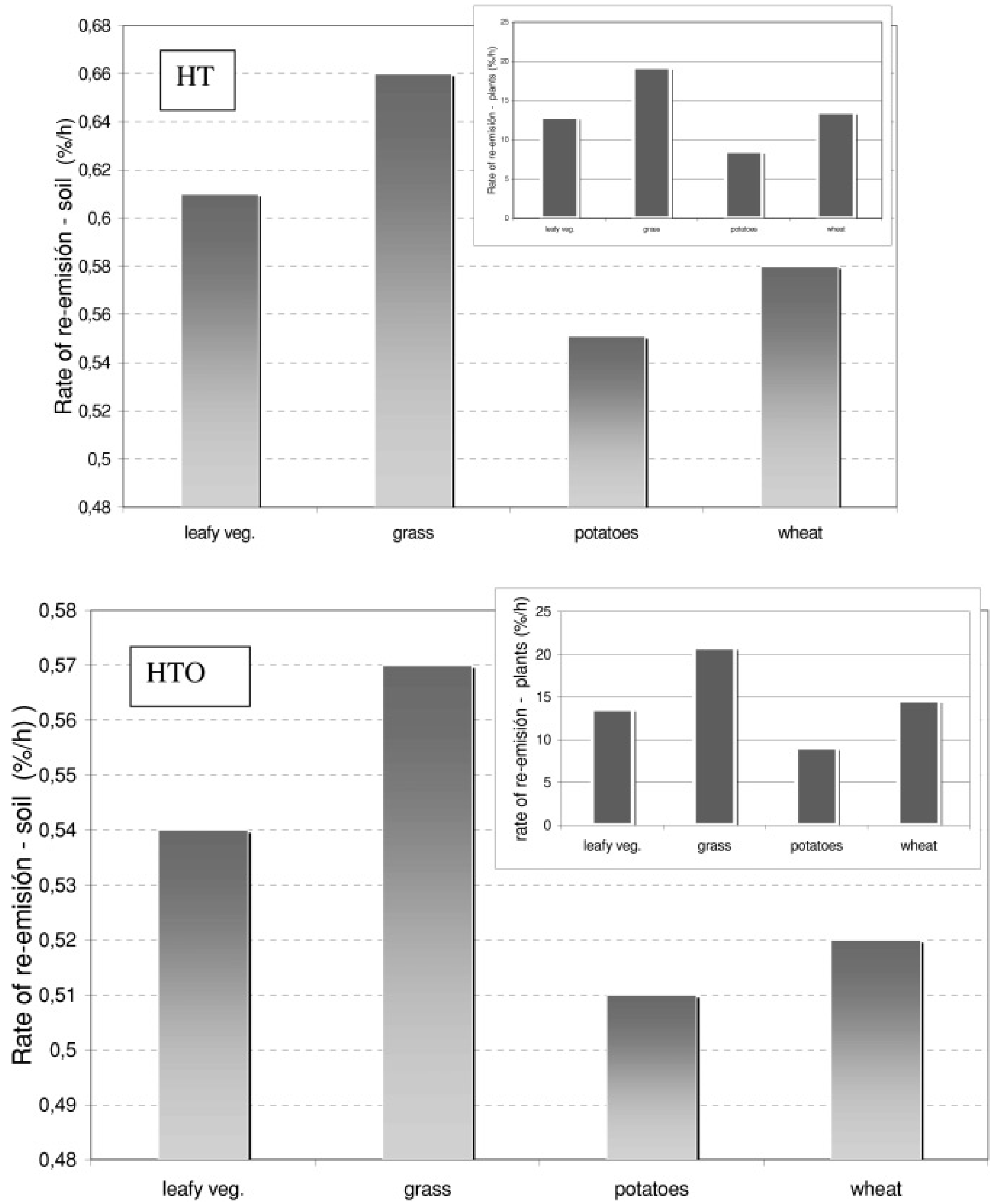

Fig. 3. Rate of Re-emission (%/h) for HT (up) and HTO (down) in four different types of vegetables with surface soil: leafy vegetables, grass, potatoes (tubers) and wheat.

of tritium transport in the environment with final consideration of different time-dependent phases in dosimetry. Our new approach allows a more realistic simulation and significant more restrictive limit in tritium handling as classically assumed in conceptual systems. This methodology was successfully used in the work performed for establishing Vandellós site for ITER (Contract under EFDA). The whole study of secondary phase drives to the conclusion that the behavior of the tritium should be simulated using two well-differentiated studies: deterministic and probabilistic. Deterministic calculations are based on a fixed meteorological data given *a priori*, where the speed and directionality of the wind, class of atmospheric stability and rain intensity, as well as the boundary conditions of the means that surround to the atmospheric discharge (soil type, humidity of the air, temperature and solar intensity) are given. The probabilistic study is based on measured real meteorological analysis every hour, and the probability that individuals can present dose for internal irradiation of the tritium is considered. Our conclusion is that these probabilistic studies provide the real dynamics of the processes, which are different from deterministic case. The effect of formation of OBT is concluded of key importance.

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