Advances in Target Design and Materials Physics for IFE at DENIM

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Abstract

A lot of work has been performed in the area related to new fuel concepts to arrive efficient cycles neutronless and p-B is the considered in our research. Conditions of degeneracy allow justifying the possibility to reduce the stringent ordinary conditions. The design of Jet Impact Inertial Fusion is one of the main items in DENIM research and simulations show a promising possibility avoiding a lot of additional technology problems; new simulations and experiments are essentially needed. Atomic Physics developments are in large progress including new models that allow simple on-line analytical expressions for target codes developments well tested with experiments. A systematic list of materials linked to their uses and area of the reactor, requirements and irradiation has been performed in order to establish the real need of adequate knowledge for qualification as low activation and change in their properties. In this paper a review of knowledge on materials under irradiation will be presented in comparison with requirements for specific purposes in IFE and MFE reactors. The first assessment need to be the nature of the irradiation particle (neutron / charged particle or radiation) depending of present ideas on reactors concepts. From that response the identification of energy spectra of secondary damage particles will be presented; in particular for optics and metallic materials. The synergy with magnetic fusion research will be highlighted and the present experiments of irradiation will be analyzed in order to have a comparative idea of usefulness of such connection. In that line a review of state-of-art of design for International Fusion Materials Irradiation Facility (IFMIF) need to be commented to know the final use for IFE purposes of such systems. The present tools of Multiscale Modeling together with *ad hoc* experiments and final macroscopic responses under irradiation will be presented in order to justify the confidence in their predictive capability to materials design.

1. Advance Fuel Cycle and degeneracy effects

Ignition temperature in classical pB11 plasmas is over 100 keV. However, in degenerate plasmas, this temperature is about 20 keV. Nevertheless, this implies to reach densities over 10^{31} electrons/cm^3 in the plasma, which is a density of 30 Mg/cm^3. It was important to complement the former work on DT fusion with a similar analysis on degenerate plasmas for proton-boron 11. The possibility to use proton beamlets of very high intensity has been explored in order to trigger the fusion onset. Extremely high currents are needed for triggering ignition (in short time of a few picoseconds) pointed out that IFE targets based on compression up to degenerate plasmas is not promising. This statement can be applied both to classical reactions and to advanced reactions (notably pB11). On the contrary, moderately high compressions in classical plasmas could offer an interesting design window to be further analysed in the context of stagnation-free implosions, complemented with impacts of plasma jets highly accelerated by the same radiation field inducing the plasma compression. This is a new way of research for alternatives targets [1].

2. Jet Impact Fusion

A new scheme for fast ignition is presented (see P. Velarde et al., this Conference, [2]) using matter accelerated to high velocity for heating the compressed DT fuel, with no additional laser to produce ignition. New EOS tables adjusted to experimental data have been implemented that automatically calculate parameters of a specially designed pressure multiplier with 5 parameters related to different physical properties, adjusting to a minimal error the Hugoniot experimental data. The NLTE package is still under testing on the multigroup radiation diffusion routines.

3. Atomic Physics Developments

Atomic physics developments for IFE targets (see E. Minguez, P. Martel et al., this Conference [3]) include: i) line photon transport in non-homogeneous plasma using radiative coupling coefficients; ii) advanced-screened hydrogenic model for opacity calculations; iii) sparse matrices techniques and iterative solvers to obtain level populations for NLTE plasmas; iv) analysis of influence of excited configurations and plasma interaction in atomic and plasma magnitudes in NLTE plasmas with analytical potential, and radiative opacity of laser-produced plasmas using relativistic-screened hydrogenic model for ions including plasma effects.

4. Safety and Environment

Many activities have been performed by DENIM devoted to the improvement of our computational methodology ACAB (see references in those included in this paper) for a reliable prediction of activation responses (references from [4] to [8]). The result is that the ACAB system is likely the worldwide most powerful tool to deal with cross section (XS) uncertainties in activation analysis. Applications of the ACAB system have focused on IFE, but also some applications are performed for IFMIF, MFE and even waste transmutation systems. The last two applications have been very useful for IFE, since activation XS needs in those fields are also closely related to some of the IFE needs. Some of the efforts are done in collaboration with USA institutions: first of all with Lawrence Livermore National Laboratory (LLNL), but also with University of California-Los Angeles, and University of Wisconsin. Collaborations with CIEMAT (Spain) and ENSTA (France) have been also initiated during this year.

The current uncertainty information on activation XS (EAF2003/05-FENDL and evaluated libraries ENDF/B-VI/VII, JENDL3.3 and JEFF-3.1) has been compiled, and conveniently processed to be used by ACAB. This XS uncertainty information is used by the ACAB code to make more reliable predictions on the isotopic inventory. The sensitivity-uncertainty approach and the Monte Carlo-based methodology are extensively used.

Isotope/Reaction	**1-energy group cross section (? in barns)**	**1-energy group cross section standard deviation (?)**	**Uncertainty in the ^{192n}Ir concentration (MSE$^{1/2}$ in %)**
^{186}W (n,?)	9.11E+00	1.04E-02	0.52
^{187}Re (n,?)	1.28E+01	1.83E-01	6.30
^{187}Re (n,?-m)	4.75E-01	1.83E-01	0.24
^{188}Os (n,?)	**6.12E+00**	**2.00E-01**	**7.87**
^{188}Os (n,?-m)	2.04E+00	2.00E-01	2.66
^{189}Os (n,n’)	9.34E-02	2.60E-01	0.00
^{189}Os (n,?)	2.25E+01	1.64E-01	3.67
^{189}Os (n,?-m)	3.46E-04	1.79E-01	0.00
^{190}Os (n,?)	**4.88E-01**	**2.72E-01**	**7.49**
^{190}Os (n,?-m)	1.15E+00	5.29E-02	3.17
^{191}Ir (n,?)	5.90E+00	1.59E-01	1.76
^{191}Ir (n,?-m)	1.23E+01	1.59E-01	3.65
^{191}Ir (n,?-n)	**3.18E-03**	**1.60E-01**	**9.94**
^{192}Ir (n,n’’)	**4.11E-02**	**2.60E-01**	**10.64**
^{192}Ir (n, ?)	4.44E+01	2.55E-01	1.19
^{192}Ir (n,?-m)	6.63E+00	2.55E-01	0.18
^{192n}Ir (n,?)	**4.44E+01**	**2.55E-01**	**17.41**
^{192n}Ir (n,?-m)	6.63E+00	2.55E-01	0.44

Table 1.- Uncertainty estimates of ^{192n}Ir build up in the ^{186}W chain due to individual cross sections uncertainties

The results presented in Table 1 clearly show the key importance of analysis using uncertainties of the cross section for some critical isotopes components of areas of IFE/MFE reactors. Here the case is the formation of ^{192n}Ir from ^{186}W that is critical as elements in fusion reactors.

Our computational tools have demonstrated to deal with the activation/transmutation issues of the intense neutron source facility IFMIF (International Fusion Material Irradiation Facility) as a first step aimed to assess its applicability to IFE needs. A comprehensive transmutation study for steels considered in the selection of structural materials for IFE reactors has been performed in the IFMIF neutron irradiation scenario. The IEAF-2001 activation library and the ACAB code were applied to the IFMIF transmutation analysis, after proving the applicability of ACAB for transmutation calculations in intermediate energy systems.

We performed the waste management assessment of the different types of steels proposed as structural material for the IFE HYLIFE-II thick-liquid concept. Both recycling options, hands-on (HoR) and remote (RR), are unacceptable. Regarding shallow land burial (SLB), 304SS has a very good performance, and both Cr-W ferritic steels (FS) and oxide-dispersion-strengthened (ODS) FS are very likely to be acceptable. The only two impurity elements that question the possibility of obtaining reduced activation (RA) steels for SLB are Nb and Mo. As concluding remarks, it seems that a reasonable liquid thickness of about 80 cm is allowable to obtain SLB acceptability of real RA steels. For a more definite answer, the uncertainties of some XS (^{94}Nb(n,?)^{95}Nb and ^{192n}Ir(n,?)^{193}Ir) should be reduced.

5. IFE Tritium Release and consequences

In the current design studies, it is indicated that the elementary tritium (HT) overcomes in some cases in one order of magnitude the effects of potential releases of tritiated water vapour (HTO). To fully simulate the behaviour of these chemical forms, we have and applied a methodology that includes diffusion and deposition processes in the soil and vegetables, the penetration in the underground, re-emission and later conversion to organic tritium (OBT). Two well-differentiated studies, deterministic and probabilistic, have been considered. Both options have been considered for a specific environment of Mediterranean location of the system. The very detailed process of re-emission has shown to be very important. It has been typically considered that the inhaled tritium is only, HTO, when, in fact part of that account is due to the HT converted to HTO and re-emitted to the atmosphere, demonstrating that HT contributes very significantly to the dose for inhalation. A dosimetric analysis of the contamination through all ways: inhalation, re-emission and ingestion have also been performed. Early and chronic doses have been evaluated. The importance of dose assessment by ingestion is more than 2 orders of magnitude if the atmospheric emission is from HTO. The significance of Dose Conversion Factors is four orders of magnitude smaller than those recommended in the regulatory guides for the HTO. This conservative overestimates the doses for the HTO, but it underestimates HT. A full detail of these advances can be found in references from [9] to [12].

6. Multiscale Modeling of Irradiated Materials

Amorphous Silica is a key component in Final Focusing of Lasers in Inertial Fusion. The energy spectra and fluxes of neutrons have been updated for different inertial fusion conceptual systems (HYLIFE-II, SOMBRERO) and magnetic fusion facilities such as ITER and IFMIF. Significant neutron moderation is obtained in the case of HYLIFE-II, and calculations were performed using materials such as PbLi and Flibe. The spectra and fluxes of other running neutron sources (HFR-Petten, BOR-60) to study radiation damage have also been considered as comparison. Primary Knock-on Atoms (PKA) energy spectra have been obtained using SPECTER code for Silica for each one of those neutron spectra. A systematic analysis of primary damage was done with TRIM and MARLOWE codes for high-energy recoils, in order to get distribution of cascades and subcascades.

We have explored hcp ?-Zirconium (very similar to hcp ?-Titanium (c/a 1.5873 for Ti and 1.593 for Zr)). It has been observed experimentally that damage produced in Zr is qualitatively similar to that in Ti. We have been researching the defect energetics and cascade damage, by using the input data obtained from molecular dynamics (MD) simulations. A systematic generation of results has been produced on irradiation of hcp ?-Zr under different conditions with a kinetic Monte Carlo model. Using 25 keV cascades we have studied the evolution of the microstructure during irradiation under environment conditions of 600K, dose rate 10^{-6} dpa/s, final dose of 0.5 dpa, and isotropic motion for vacancies. How the accumulation of damage is affected considering interstitial movement from one dimension to three-dimension has also been studied.

Concerning ferritic steeels, new diffusion parameters from *ab-initio* calculations were implemented in kinetic MonteCarlo BIGMAC code. 150 keV Fe^{+} ion irradiation in UHP-Fe were developed. Simulations were performed using the new activation energies and 3D motion for the diffusion of interstitial defects. New vacancy's migration energies for 3-4 vacancy clusters and last *ab-initio* diffusion parameters for impurities were also implemented. TEM observations at CIEMAT were developed to quantify the defect concentration and the defect type. Large differences between old and new parameters and between simulations and experiments have been observed (from 350 nm in experiments to 8 nm in simulations). New mechanisms have been proposed to explain those differences, such as new reaction probabilities and surface effects. Dislocation Dynamics has been used to study the interaction of Stacking Fault Tetrahedra (SFT) with Partial dislocation successfully using Lawrence Livermore National Laboratory code DD3D and PARADIS. The generation of SFT has been demonstrated computationally at the same time that the key importance of the equivalent modeling of mesoscopic scale and atomistic when describing defects-dislocation interaction in fcc materials such as Cu.

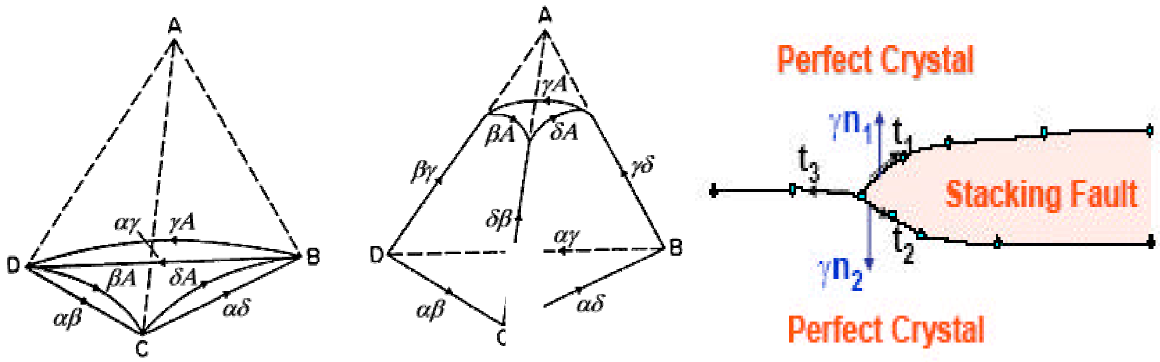
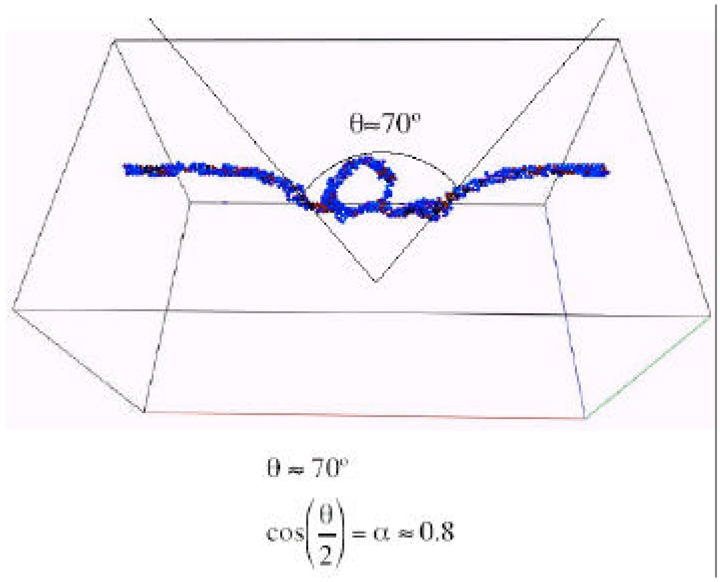


Figure 1.- The formation of SFT fron. .'rank loop has been clearly demonstrated as expected theoretically by using dislocation dynamics and partials interaction in it. That explains mechanisms in fcc materials to be now extended to bcc (such as Fe) which is a new step at the mesoscopic scale in multiscale modeling.



In this Figure 2 we demonstrate use of Molecualr Dynamics simulation in obtaining stress-strain characteristics.Stress computed using *Orowan* theory is 590 Mpa; that is an error with experiments of only 50 % [26].

Molecular Dynamics Simulations study of damage as a consequence of displacement cascades due to energetic recoils in fused silica have been performed. We have identified and characterised defects in fused silica using several methodologies. To characterise a defect we have analysed a simulation box with different stoichiometry in order to make observations of how those defects interact with the nearest neighbours. In addition, we have made displacement cascade study in order to look which is the behaviour of defects in the cascade evolution with the goal to understand better the different kind of defect that they are generating in the fusion reactor environment. The range of primary knock-on atom (PKA) energy studied in this moment is from 20 eV to 3.5 eV.

Previous described work in different areas is done in references from [13] to [25].

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8. References

[1] P. Leon, S. Eliezer, J.M. Martínez-Val, Physics Letters A 343 (2005) 181-189.
[2] P. Velarde et al., 21st IAEA Fusion Energy Conference, 16-21 October 2006, Chengdu, China
[3] E. Minguez, P. Martel, et al., 21st IAEA Fusion Energy Conference, October 2006, Chengdu
[4] O. Cabellos, S. Reyes, J. Sanz, A. Rodriguez, M. Youssef, M. Sawan, Effect of Activation Cross Section Uncertainties on the Radiological Assessment of the MFE/DEMO First Wall, 7th International Symposium on Fusion Nuclear Technology, Tokyo (Japan), May, 2005
[5] O. Cabellos, J. Sanz, N. García-Herranz, S. Díaz, S. Reyes, S. Piedloup, Transmutation Analysis of Realistic low-Activation Steels for Magnetic Fusion Reactors and IFMIF, 12th International Conference on Fusion Reactor Materials, Santa Barbara (USA), December, 2005
[6] O. Cabellos, J. Sanz, N. García-Herranz, S. Díaz, S. Reyes, S. Piedloup, Transmutation Analysis of Realistic low-Activation Steels for Magnetic Fusion Reactors and IFMIF, 12th International Conference on Fusion Reactor Materials, Santa Barbara (USA), December, 2005
[7] J. Sanz, O. Cabellos, S. Reyes, Effect of activation cross-section uncertainties in selecting steels for the HYLIFE-II chamber to successful waste management, Fusion Engineering and Design 75–79 (2005) 1157–1161
[8] O. Cabellos, J. Sanz, S. Reyes, N. García-Herranz, Waste management sensitivity analysis in different neutron environments for IFE thick-liquid concepts, International Conference on Inertial Fusion Sciences and Applications, Biarritz (France), Septiembre, 2005.
[9] J.M. Perlado, J. Sanz, M. Velarde, S. Reyes, M.J. Caturla, C. Arévalo, O. Cabellos, E. Domínguez, J. Marian, E. Martínez, F. Mota, A. Rodríguez, M. Salvador, G. Velarde, Activation

and Damage of Fusion Materials and Tritium effects in Inertial Fusion Reactors: strategy for adequate irradiation, Laser & Particle Beams (2005) 23, 345-349.
[10] W. Raskob, M. Velarde, J.M. Perlado, Tritium Dose Assessments With Regulatory And Advanced Computer Models For The Potential European Iter Site Vandellós (Spain), Fusion Science and Technology, vol 48 n1 (2005), p 492-495.
[11] M. Velarde, J.M. Perlado, L. Sedano, Behaviour of Three Chemical Forms of Tritium in the Environment after Release from Inertial Fusion Reactors, Published in Book Inertial Fusion Science and Applications, IFSA 2005 (2005)
[12] J.M. Perlado, J. Sanz, M. Velarde, O. Cabellos, C. Arévalo, N. García-Herranz, E. Martínez, F. Mota, S. Reyes, M.J. Caturla, J. Marian, G. Velarde, M. Victoria, P. Cepas, M.L. Gámez, Inertial Fusion Reactor Physics: effect of Activation and Radiation Damage of Materials, and Tritium emissions. Presented and published in Book of EPS Fusion Conference 2005, Tarragona, June 2005
[13] J.M. Perlado, J. Sanz, M. Velarde, S. Reyes, M.J. Caturla, C. Arévalo, O. Cabellos, E. Domínguez, J. Marian, E. Martínez, F. Mota, A. Rodríguez, M. Salvador, G. Velarde, Activation and Damage of Fusion Materials and Tritium effects in Inertial Fusion Reactors: strategy for adequate irradiation, Laser & Particle Beams (2005) 23, 345-349.
[14] C. Arévalo, M.J. Caturla, J.M. Perlado, Long-term behavior of irradiated hcp Zr using MonteCarlo simulations, Nuclear Instruments and Methods in Physics Research B (2005) 176-180.
[15] F. Mota, M.J.Caturla, J.M.Perlado, E.Dominguez , A. Kubota, Threshold energy of formation of an oxygen vacancy defect in SiO_2 by atomic displacements using molecular dynamics, Fusion Engineering and Design, 75-79 (2005) 1027-1030
[16] C. Arévalo, M.J. Caturla, J.M. Perlado, Temperature dependence of damage accumulation in hcp metals., Accepted for publication in Journal if Nuclear Materials (2006)
[17] F. Mota, J,M. Perlado et al., Identification and characterization of defects produced in irradiated fused silica through molecular dynamics, Accepted for publication in Journal of Nuclear Materials (2006)
[18] J. Mollá, F. Mota, M. León, A. Ibarra, M.J. Caturla J.M. Perlado,, The role of the fused silica stoichiometry on the intrinsic defects concentration, Accepted for publication in Journal if Nuclear Materials (2006)
[19] F. Mota, J.M. Perlado, et al., Thermal stability of neutron irradiation effects on KU1 fused silica, Accepted for publication in Journal if Nuclear Materials (2006)
[20] M. L. Gámez, M. Velarde, F. Mota, J. M. Perlado, M. León, A. Ibarra, PKA energy spectra and primary damage identification in amorphous silica under different neutron energy spectra. Accepted for publication in Journal if Nuclear Materials (2006)
[21] J.M. Perlado, M. Victoria, M.J. Caturla, J. Marian, M.L. Gámez, C. Arévalo, E. Martínez, F. Mota, M. Velarde, G. Velarde, P. Cepas, Radiation Damage in Metals, and Amorphous Silica in Inertial Fusion Reactors: Modeling and Experiments. Published in Book Inertial Fusion Science and Applications, IFSA 2005 (2005)
[22] J.M. Perlado, J. Sanz, M. Velarde, O. Cabellos, C. Arévalo, N. García-Herranz, E. Martínez, F. Mota, S. Reyes, M.J. Caturla, J. Marian, G. Velarde, M. Victoria, P. Cepas, M.L. Gámez, Inertial Fusion Reactor Physics: effect of Activation and Radiation Damage of Materials, and Tritium emissions. Presented and published in Book of EPS Fusion Conference, Tarragona, June 2005.
[23] E. Martínez, J.M. Perlado, M.Victoria, M.J.Caturla, P.Cepas, J.Marian, D.Gomez, M.Hernandez Microstructure simulation of radiation damage in metals using improved kinetic

Monte-Carlo defects diffusion modeling', in Proc. Micromechanics and Microstructure evolution: modeling, simulation and experiments, Madrid, September 2005.
[24] E. Martínez, J.M. Perlado, M.Victoria, M.J.Caturla, P.Cepas, J.Marian, D.Gomez, M.Hernandez, Accumulation damage in Fe using kinetic MonteCarlo implemented with the last *ab-initio* parameters, in Proc. Micromechanics and Microstructure evolution: modeling, simulation and experiments, Madrid, September 2005.
[25] E. Martínez, J. Marian, A. Arsenlis, M. Victoria, J.M. Perlado, Atomistically-informed Dislocation Dynamics in fcc Crytals, presented at European Materials Research Society (EMRS) (2006), to be submitted to Solid State (2006).
[26] J. Marian, B, Wirth, B. Odette, R. Schaublin,, J.M. Perlado, J. Muclear Materials (2003)