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INDC International Nuclear Data Committee

Summary Report of
the First Research Coordination Meeting on
Primary Radiation Damage Cross Sections

IAEA Headquarters, Vienna, Austria
4 – 8 November 2013

Prepared by
R.E. Stoller, Oak Ridge National Laboratory, Oak Ridge, TN, USA
L.R. Greenwood, Pacific Northwest National Laboratory, Richland, WA, USA
S.P. Simakov, Nuclear Data Section, IAEA, Vienna, Austria

December 2013

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

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Abstract

The Nuclear Data Section of IAEA has initiated a new Coordinated Research Project with the main goal of reviewing and recommending primary damage response functions for neutron and ion irradiations of materials. The output of this CRP will be a database of recommended damage response functions for selected materials with corresponding documentation. It will serve the needs of the fission, fusion and accelerator neutron source communities. The first Research Coordination Meeting (RCM) was held 4 to 8 November 2013 at the IAEA. At this meeting, the attendees discussed the objectives of the whole CRP, presented their contributions and elaborated on consolidated recommendations and actions for implementation over the next 1.5 year period. This Summary Report documents the individual contributions and joint decisions made during this meeting. The identified research needs were refined through extensive discussion, and a consensus was developed which defined the CRP objectives in two broad categories. The first addresses the underlying physics-related research relevant to nuclear reactions and ion stopping powers, while the second task will address the development of new materials damage response functions.

December 2013

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I. Introduction

Motivation, objectives and outcomes of the IAEA Coordinated Research Project

The Nuclear Data Section of the IAEA, in accordance with the recommendation of the International Nuclear Data Committee (INDC) meeting held in May 2012 [1] and the Technical Meeting "Primary Radiation Damage Cross Sections" held in October 2012 [2], has initiated a new Coordinated Research Project (CRP number F44003). The first Research Coordination Meeting (RCM) was held 4 to 8 November 2013 at the IAEA. The background, purpose, and objectives of the CRP are discussed below.

When materials are exposed to irradiation by energetic particles, two types of parameters are used to characterize the cumulative exposure of a material, *viz.* particle fluence and absorbed dose. The particle fluence, in units of particles/unit area, depends only on the characteristics of an irradiation source and can be quoted at a point or averaged over a surface or volume. The absorbed dose, in units of energy, depends on a variety of variables, including: particle fluence, particle type, particle energy spectrum, and the specific material being exposed. Thus, absorbed dose is influenced by a wide range of characteristics of the irradiation environment, and it is material dependent. Both particle fluence and absorbed dose can be used to correlate data which describes some measured effect of irradiation. Use as a damage correlation parameter entails a much broader range of influences than simply the material and the irradiation source. In general, the application of a damage correlation parameter will depend on: the particle fluence or absorbed dose, specific damage parameter being monitored (e.g. electrical resistivity, swelling, or embrittlement), the damage rate, previous damage, exposure conditions such as temperature and mechanical loads, and material composition (intentional alloy elements, dopants, and impurities). The impact of correlated damage mechanisms such as transmutation reactions, notably the creation of helium and hydrogen, must also be considered.

Since its introduction in 1975, the secondary displacement model of Norgett, Robinson, and Torrens (NRT) has been a de facto dosimetry standard in the nuclear materials research community [3]. The NRT model provides a procedure for estimating the number of atomic displacements per atom (dpa) due to the kinetic energy the atoms in a material absorb during exposure to high energy particles, the so-called damage energy. The damage energy is obtained from fundamental physics data and (most commonly) the energy partitioning theory of Lindhard, et al. [4]. For a given primary knock-on atom (PKA), a range of elastic and inelastic collisions may contribute to the damage energy. An accurate calculation of damage energy is specific to the energy spectrum of the incident irradiating particles and requires the nuclear data necessary to obtain a good representation of the PKA recoil spectrum in the material of interest. Interatomic potentials are required to characterize the partition of energy for the recoiling PKA between various electronic and nuclear energy loss mechanisms. Modern molecular dynamics (MD) simulations and cryogenic irradiation experiments clearly indicate that the number of stable vacancies and interstitials formed in irradiated materials is about 20 to 40% of the NRT value [5]. Alternate materials damage response functions have been developed that appear to provide a better estimate of stable Frenkel pair production in iron, as well as other damage parameters related to in-cascade clustering [6, 7].

The CRP work is currently planned for the time period from 2013 through 2017. The main CRP outputs will be the damage response functions, NRT- and PRD- (also called athermal recombination-corrected) dpa as well as gas production cross sections and their uncertainties in a numerical database. The CRP final document will describe the database and the results of research. Additional information is available on the CRP web-page https://www-nds.iaea.org/CRPdpa/.

The first Research Coordination Meeting (RCM)

The 1st RCM of the new IAEA CRP on "Primary Radiation Damage Cross Sections" was held at IAEA Headquarters, Vienna, Austria from 4 to 8 November 2013. The following holders of the CRP Research Agreements have attended this meeting: I. Bondarenko, O. Cabellos, M. R. Gilbert, U. Fischer, P. Griffin, Y. Iwamoto, A. Kahler, A. Konobeev, L. Luneville, F. Mota, K. Nordlund,

D. Simeone, J.-C. Sublet, R. Stoller, D. Terentyev and C. Woo. M. Catutla, A. Koning, R. Vila, and J. Kwon could not attend. L. Greenwood, D. Leichtle and L. Ping took part as observers. The Nuclear Data Section of IAEA was represented by S. Simakov (Project Officer), R. Forrest (Alternative Project Officer), N. Otuka, and V. Semkova.

The Meeting was opened by M. Venkatesh, Director of Division of Physical and Chemical Sciences of the Department of Nuclear Sciences and Applications of the IAEA, who welcomed the participants and stressed the importance of this CRP for establishing well defined metrics and reference data for radiation damage in the structural materials used as in nuclear applications.

A. Öchs, who is responsible for administrative issues, made several announcements. This was followed by the self-introduction of participants.

The participants elected R. Stoller as the Chairman and L. Greenwood as the Rapporteur of this Meeting and approved the Agenda for the meeting (Appendix I). The list of participants and their affiliations are summarized in Appendix II.

The objective and goals of the Meeting were outlined by S. Simakov.

During the first Research Coordination Meeting of the Coordinated Research Project for Primary Radiation Damage Cross Sections, the participants made seventeen technical presentations (they are available on the CRP web page) which provided a description of research needs identified by each presenter, along with the scope of work that they were prepared to carry out in the context of the CRP. The identified research needs were refined though extensive discussion, and a consensus was developed which defined the CRP objectives in two broad categories as described below.

The discussions resulted in a set of consolidated conclusions, recommendations and actions (Section II). The summaries of the CRP participants' presentations and planned work in frame of CRP are collected in Section III.

The Nuclear Data Section acknowledged all participants for their cooperation and contributions to the Meeting.

II. Summary of Meeting Recommendations with Action Items

Based on the presentations by CRP participants and their subsequent discussion, the work scope of the CRP was determined to lie in two broad categories. The first is related to the underlying physics of interactions between energetic particles and will specifically address research relevant to nuclear reactions and ion stopping powers. The principle outputs of this task will be primary knock-on atom spectra and damage energies. Based on the results of the first component, the second task will address the development of materials damage response functions. In the following sections, the work scope identified for both tasks is summarized and lists of action items identify the participants involved in carrying out the work.

Nuclear Reactions and Ion Stopping Data

The participants agreed that the most fundamental radiation damage parameters are the primary recoil atom spectra and the damage energy. All other damage response functions are derived from these basic quantities. Consequently, the CRP should produce a database for selected materials that provides a community consensus of the best values for these quantities.

The primary recoil spectra are calculated from reaction models and using the energy dependent nuclear interaction cross sections and angular distributions. It was recommended that ENDF/B-VII.1 [11] was the most complete source of nuclear cross sections and should be augmented with the latest version of TENDL [11] cross sections as needed to account for all possible nuclear reactions, especially at higher neutron energies. Other nuclear data libraries should also be used in specific cases such as gas production.

The energy of the primary recoil atoms is partitioned into electronic and nuclear stopping using the LSS theory [4]. The sum of the nuclear stopping power for all possible recoils is defined as the damage energy and this is the most fundamental quantity of radiation damage in most structural materials. The NJOY-2012 [12] computer code is recommended for performing these calculations to create the damage energy libraries. Uncertainties and covariances should be included in these databases when possible.

The energy range of interest is from 0 to around 3 GeV in order to include experiments conducted not only in fission reactors, but also at particle accelerators such as spallation neutron sources, and the proposed IFMIF for the study of fusion reactor materials. However, the existence of suitable quality data may restrict the library to 150 MeV. Evaluated data, based on experimental data, are used where available; extensive experimental data are available for neutrons below 20 MeV with more limited data up to ~150 MeV. Below ~150 MeV, direct and compound nuclear reaction models based on optical model potentials are used to augment the available experimental data. For higher neutron energies the nuclear reaction data are best derived from codes that use intranuclear cascade (INC) models such as those incorporated into the PHITS code. NRT and arc-dpa and gas production cross sections for Al, Ti, V, Cr, Cu, Zr already exist in the DXS library [13] for neutrons and protons up to 3 GeV.

A number of issues relevant to the development of the cross section libraries were discussed. With respect to damage partitioning, Robinson's fit to general LSS theory [4] is only valid when the recoil and matrix atoms have similar masses. The more general LSS theory must be solved for other cases. Based on the seminal work of Lindhard, et al. [4], the repartition of this damage energy for different species of various masses has been achieved [5,6]. The DART code was developed to determine the energy damage partitioning in polycristalline materials from neutron libraries [7]. The DART code may be used to accurately compute the energy partitioning using the full LSS model.

The use of NJOY-2012 [12] to obtain PKA spectra and damage energy for the range of materials of interest to the CRP may require some modification of this code in order to include updated recoil ion energy partition functions. Care must be taken in interpreting recoil atom spectra when, at discrete energies, the evaluated nuclear cross section files may change the format used to characterize the cross

section data. Some apparent discrepancies in PKA spectra obtained when processed using different nuclear data libraries were shown by A. Konobeyev and need to be investigated.

Action items:

- Determine and provide recommendations for the correct processing of PKA spectra and damage energy functions and investigate discrepancies between different libraries and different processing steps [O. Cabellos, Y. Iwamoto, A. Konobeyev, S. Simakov, J.-C. Sublet, A. Kahler, J. Kwon, M. R. Gilbert, P. Griffin]
- Propagation of uncertainties of PKA spectra, displacement threshold energy, etc. to the damage energy [O. Cabellos, A. Konobeyev, A. Koning, P. Griffin]
- Investigation of the uncertainty of damage functions in semiconductor materials Si, GaAs [P. Griffin]
- Employ the DART code to determine the energy partitioning for polyatomic materials such as SiO_2 and Al_2O_3 and SiC. [D. Simeone, L. Luneville]
- Prepare figures for the final report showing the PKA energy distributions for Fe, Zr, and SiC for different radiation environments (1/4 T RPV, HFIR, PTP, ITER first wall, DEMO, PHENIX, SNS, IFMIF) [Y. Iwamoto, F. Mota, J.-C. Sublet, M.R. Gilbert]
- Damage response functions [L. Luneville, J. P. Crocombette, J.-C. Sublet]
- Modification of NJOY as needed (possibly experimental versions) [A.C. Kahler]
- Investigate differences in the implementation of the Robinson formula for energy partition using the LSS theory between MCNP/HTape3x and NJOY [A. Konobeyev]

Transmutant gas production (hydrogen and helium) produced by neutrons and protons is also of fundamental importance in the evolution of radiation damage and should be included in the database. The GASPR module of NJOY-2012, which sums over all possible neutron reactions leading to either H or He, will be used with the ENDF/B-VII.1 database and may be augmented with TENDL to supply any missing reactions to provide an updated gas production database.

Uncertainties and covariances for the gas production should also be addressed and the energy range should match that of the damage energy functions. The CRP includes some new measurements of gas production on some elements (Cr and Fe isotopes) in the 5 to 7 MeV energy range supplied by I. Bondarenko of the IPPE.

In some situations, solid transmutation products can also be very important in the damage evolution of irradiated materials. Depending on the specific material cross sections, either thermal or high energy neutrons may more important. The final report of the CRP should address this issue with some discussion of the most important issues, although including such calculations in the database was deemed to be outside of the scope of the CRP.

Action items:

- Intercomparison and recommendation for gas production cross sections available in the evaluated files and nuclear reaction models at higher energies [J.C. Sublet, A. Konobeyev, S. Simakov, O. Cabellos, A. Koning, Y. Iwamoto]
- Assessment of uncertainties in gas production [O. Cabellos, A. Koning]
- Gas production experimental data for Cr and Fe in the 5 to 7 MeV neutron energy range [I. Bondarenko, IPPE]
- Discussion of the importance of solid transmutation [L.R. Greenwood, R.E. Stoller, J. C. Sublet, M.R. Gilbert]

Development of Materials Damage Response Functions

As stated above, the NRT model has been a *de facto* standard materials damage response function since the mid-1970s. The model provides one way of converting damage energy to an estimate of the number of atomic displacements per atom (dpa) due to material irradiation by high energy particles. The most extensive databases of MD displacement cascade simulations that provide a better estimate of stable Frenkel pair production have focused on iron or simple iron-based binary alloys. Within the CRP, this work will be extended to a broader range of materials and additional damage response functions.

Existing databases of molecular dynamics cascade simulations will be employed and augmented by members of the CRP. The target materials are listed in Table 1.

Table 1: List of materials and CRP members involved in MD for damage response functions

Fe, Fe-xCr, Fe-Ni, Fe-Ni-Cu-Mn, Ni, Cr, Mn	K. Nordlund, R. E. Stoller, M. Caturla, J. Kwon, D. Terentyev
Zr	K. Nordlund, R. E. Stoller
W	K. Nordlund, R. E. Stoller
Cu, Ag, Pd, Pt	K. Nordlund, R. E. Stoller
SiC	K. Nordlund, R. E. Stoller, D. Simeone
SiO_2 and Al_2O_3	K. Nordlund, F. Mota, C.J. Ortiz, R. Vila, D. Simeone
ZrC and UO_2	J.P. Crocombette, L. Van Brutzel

Analysis of the MD simulations employing the nuclear data results from the first task will lead to the development of new damage response functions for selected materials. The new damage response functions to be included in the database include: total defect survival, which accounts for athermal recombination, surviving interstitials in clusters, surviving vacancies in clusters, and measures of the point defect cluster size distributions. Applicability of damage response functions for polyatomic ordered compounds will be checked.

These functions will be evaluated based on experimental data already in the literature and new cryogenic defect production experiments being conducted in Japan using the FFAG accelerator facility (150 MeV protons) in the Kyoto University Research Reactor Institute. Their use as damage correlation parameters will be assessed using historical examples in which the NRT dpa was previously employed, such as the ORNL HFIR pressure vessel [15], the UK Magnox reactor pressure vessels [16], and specific data sets that include multiple irradiation environments such as that in Ref. [17].

Action items:

- Fitting and evaluation of MD-based materials damage response functions [R. E. Stoller, K. Nordlund, L. R. Greenwood, J. P. Crocombette]
- Experimental measurement for cryogenic defect production is planned using the 150 MeV proton beam at the FFAG accelerator facilities at the Kyoto University Research Reactor Institute [Y. Iwamoto]

Codes employing the binary collision approximation (BCA) are commonly also used to investigate primary damage formation. The CRP will include specific items of research concerning the relationship between BCA and MD simulations.

Action items:

- MD-based parameterization of the BCA recombination radius for silica and alumina [F. Mota, C.J. Ortiz, R. Vila, K. Nordlund]
- implementation and use of an integrated BCA-MD code for cascade simulations in Fe and Zr [A. Konobeyev]
- BCA simulations of displacement cross sections for polyatomic ceramic materials Li_2O, Li_4SiO_4, Li_2TiO_3 [D. Leichtle]

The final report will include a discussion of a number of other topics that influence the production or short-term evolution of radiation damage in materials although they are not directly included in the research activities of this CRP. The list of such items and the participants responsible for providing the relevant information are listed below.

Action items for final report:

- cascade aging [R.E. Stoller, M. Caturla]
- effects of magnetism, spin dynamics [Chung Woo]
- thin films [M. Caturla, R. E. Stoller]
- comparison of ion and neutron irradiations, PKA spectra, cascade evolution [R. E. Stoller, L.R. Greenwood, M. Caturla]
- cascade size [C. Woo]

Finally, radiation damage parameters such as the NRT dpa and gas production have been used for many years and there is a large literature including materials handbooks and regulatory guides based on such quantities. It is thus deemed essential that the relationship of any new damage response functions parameters produced during this CRP be discussed in the context of previously used parameters in order to maintain continuity with the very large literature that is available for materials research.

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III. CRP Participants Summaries

Nuclear data for fusion applications: dpa beyond NRT?

Dieter Leichtle

ITER, Department Fusion for Energy
Barcelona
Spain

Introduction

The European Union has established Fusion for Energy, the Joint Undertaking for ITER and the Development of Fusion Energy, with a threefold mission, namely to provide the EU contribution to ITER, to implement EU contributions to the Broader Approach activities, and also to coordinate R&D in support of a DEMO fusion reactor. Qualified computational tools and data have to be provided for reliable nuclear analyses in support of the design, construction, licensing, operation and safety case of fusion devices like ITER and DEMO. As an integral part of its project plan, F4E has set up a Nuclear Data Project which covers both theoretical and numerical (nuclear data evaluation, processing and benchmarking), as well as experimental (measurements and experimental validation) activities. It is implemented by Framework Partnership Agreements (FPA) with two nuclear data consortia, formed by European research institutions. The overall objective of the R&D activities conducted in the Nuclear Data Project is to support the development and validation of predictive capabilities, including reliable uncertainty margins, of nuclear analysis tools.

Within the current grant activities two tasks are devoted to primary radiation damage cross sections, which fit nicely into the CRP on this topic. One action is on providing a complete dpa (displacement per atom) cross section library for applications with the MCNP code using state-of-the-art nuclear data libraries and standard dpa models. The second action is on improved dpa cross sections for main elements of the RAFM steel EUROFER. It encompassed advanced dpa models utilizing results from BCA and MD simulations. The leading scientists are contributing to the CRP and provide individual sections in the Report from the 1st RCM.

Primary damage correlation and standard NRT

The strong 14 MeV neutron source of a DT fusion device gives rise to a severe radiation environment, particularly for the components close to the plasma source. The neutron exposure causes material degradation which has to be predicted in order to assess performance and anticipated life-time of the irradiated components. To this end, irradiation experiments on candidate materials are conducted to study material properties under irradiation up to the relevant levels. In order to quantify and compare different irradiation conditions suitable damage correlation parameters are needed. The number of stable lattice defects (interstitial atoms, vacancies) surviving the quenching of the collision cascade initiated by a primary knock-on atom (PKA) can establish a fundamental input for such parameters.

The most often applied parameter is the rate of displacements per atom (dpa). It combines the probability for the production of PKAs and the number of defects created by each PKA, integrating over the irradiation particle flux spectrum. One derived quantity, the damage-weighted cumulative PKA-spectrum, has been used frequently by many authors. The reason for this is, that it is superior to the comparison of bare total dpa in different neutron spectra as it includes in addition the resulting spectrum of PKA. In terms of qualitative judgement, the shape and mass distribution of PKA spectra are considered as the most important and meaningful quantities.

Based on the concept of damage energy (the share of the PKA kinetic energy, which is transferred to secondary knock-on atoms and responsible for displacing atoms) the standard NRT model [2] of displacement damage has been used now commonly for a wide range of materials. It has been adopted as a general reference, albeit well-known deficiencies in its physics, applicability and interpretation regarding the primary damage state. Addressing these issues and/or replacing the “standard” by a new

damage model is needed and welcomed; but it is believed, that this should lead inevitably to proposing and finally adopting a new "standard".

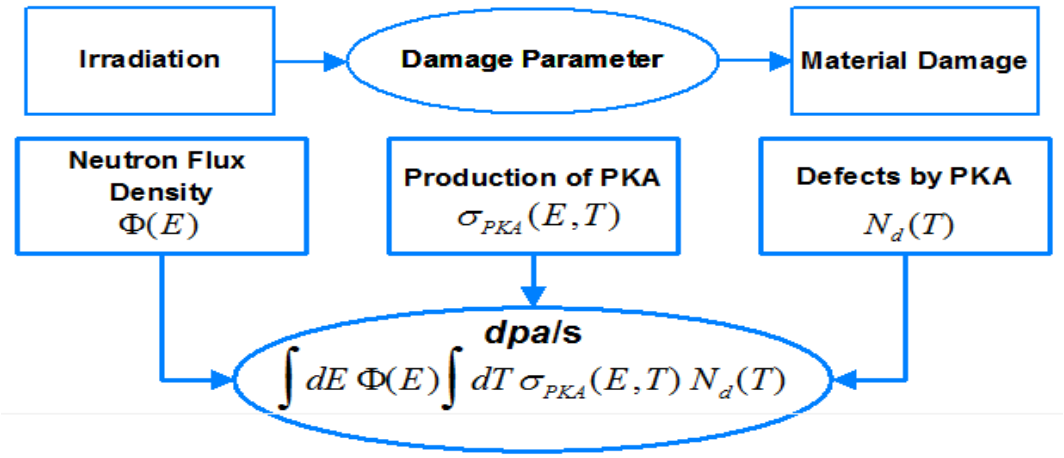

Fig. 1: Scheme of primary damage correlation by dpa.

Some aspects of NRT deficiencies

To elucidate one area of NRT deficiencies, the case of light-mass and polyatomic materials will be detailed in the following on the example of breeding blanket materials, namely Beryllium and Lithium ceramics. In this case, a broad range of PKA masses (from Tritium and Helium to e.g. Titanium) and energies (up to several MeV) have to be taken into account.

Based on BCA simulations using a local version of the Marlowe-Code [6], which specific updates relevant to this class of materials (see [1]), several distinguished aspects can be identified. Firstly, the morphology of resulting defects is quite different to the classical dense cascades seen in metals. Secondly, although the damage energy concept is confirmed, a further increase at higher energies is observed due to updated electronic stopping powers. And finally, the effective threshold energies in different sublattices do depend on PKA type and energy which complicates the adoption of a single, averaged value in the standard NRT model.

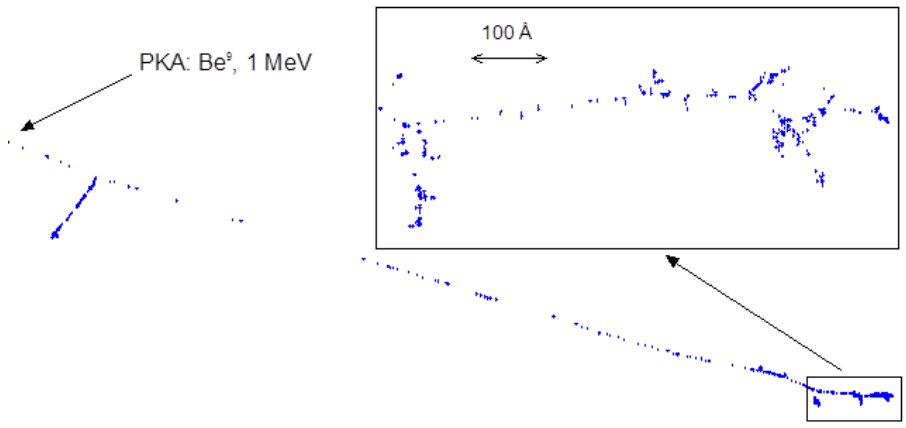

Fig. 2: BCA cascade of 1 MeV Be PKA in Be, showing dilute Frenkel pair production.

Neutron spectra effects can be seen in the PKA spectrum, particularly for Tritium and Helium from the ^{6}Li(n,t) reaction which dominates at low neutron energies. This difference develops into the contributions of those PKAs to the total damage, which can be utilized to tailor the neutron (and therefore also the PKA) spectrum in an irradiation experiment.

Utilizing improved displacement cross sections for this class of materials based on the aforementioned BCA simulations one can derive grossly altered dpa values (see e.g. [3], [4], [5]). In the case of

Beryllium an increase by 90% in a fusion First-Wall spectrum has been obtained, due to mainly enhanced defect production by Helium atoms from (n,2n) and (n,α) reactions. For Lithium silicates, on the contrary, a reduction of about 30% is seen. This stems from effects of the crystalline structure which generally tend to suppress the formation of stable defects. However, for a thermal neutron flux, where contributions from light-mass PKA are dominating the enhanced damage from those would lead to a general increase in dpa.

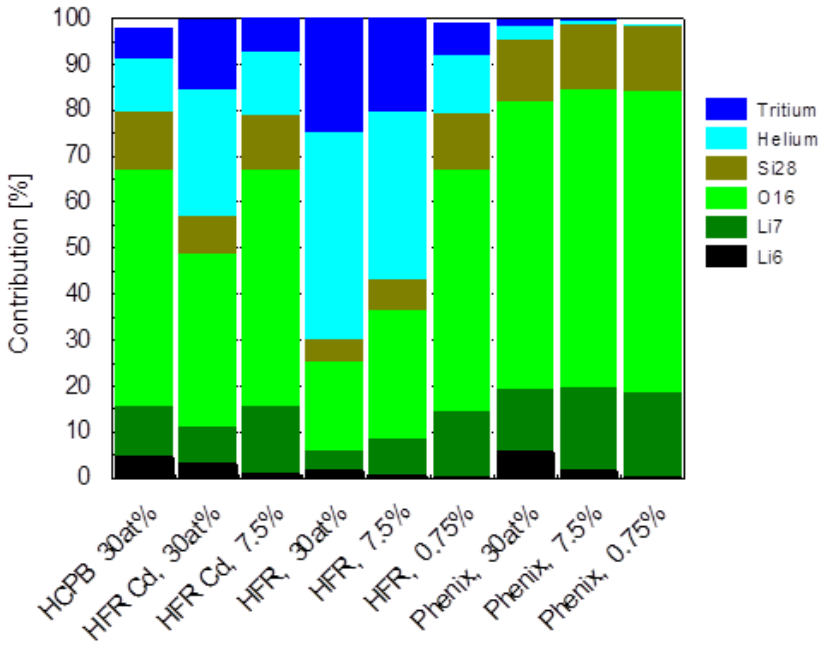

Fig. 3: PKA contributions to total dpa for different neutron spectra (Lithium silicate)

Summary

Fusion for Energy is providing nuclear data and nuclear analysis support to EU fusion projects. It is focusing on reliable, validated, and standardized reference data and tools. Primary radiation damage parameters (DPA) for quantifying material damage effects in different irradiation conditions are of ultimate importance to properly qualify candidate materials for fusion reactor design, operation and licensing. The need for improvement or replacement of the standard NRT model of dpa is conceived, but going beyond standard DPA-NRT would inevitably require going to a new standard.

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Primary Radiation Damage in metals

Kai Nordlund

University of Helsinki
Finland

1. Overview of OECD dpa group work.

We have scientifically finalized the OECD Nuclear Energy Agency Primary Radiation Damage (PRD) group report. This report reviews the current understanding of primary radiation damage from neutrons, ions and electrons (excluding photons, atom clusters, and more exotic particles), with emphasis on the range of validity of the dpa concept in all main classes of materials (except organic ones), and in particular discuss known shortcomings. The report describes that the current NRT-dpa standard is fully valid in the sense of a scaled radiation exposure measure, as it is essentially proportional to the radiation energy deposited per volume. As such, it is highly recommended to be used in reporting neutron damage results to enable comparison between different nuclear reactors and ion irradiations. However, in the sense of a measure of damage production the NRT-dpa value has several well known problems, which are discussed at length.

To partially start to alleviate these problems, for the case of metals the report present an "athermal recombination-corrected dpa" (arc-dpa) equation that accounts in a relatively simple functional for the well known issue that the dpa overestimates damage production in metals under energetic displacement cascade conditions, as well as a "replacements-per-atom" (rpa) equation that accounts in a relatively simple functional for the well known issue that the dpa severely underestimates the actual atom relocations (ion beam mixing) in metals.

The report also presents a recommendation for how the dpa value for ion irradiation conditions should be obtained from the widely used SRIM binary collision approximation code.

The OECD report provides a scientific motivation and functional forms for a modified "athermal-recombination-corrected" arc-dpa to describe damage production in metals as well as a "replacements-per-atom" function to describe ion beam mixing. The arc-dpa and rpa functions are identical to the NRT-dpa at the threshold, but differ above it. The threshold energy used in arc-dpa is to be the same as in the NRT-dpa, but in addition the function uses two more element-specific parameters that provide information on the so called damage efficiency that tells how much less damage is produced than the NRT equation predicts.

The report provides initial parameters for the arc-dpa function for Fe and for the rpa function for Ni, Pd and Pt. After some polishing of the text, a preprint of the report will be distributed to the IAEA CRP members.

2. Damage production in W

Recent experiments on in situ high-energy self-ion irradiation of tungsten (W) show the occurrence of unusual cascade damage effects resulting from single-ion impacts, shedding light on the nature of radiation damage expected in the tungsten components of a fusion reactor. We have investigated the dynamics of defect production in 150 keV collision cascades in W at atomic resolution, using molecular-dynamics simulations and comparing predictions with experimental observations. We showed that cascades in W exhibit no subcascade break-up even at high energies, producing a massive, unbroken molten area, which facilitates the formation of large defect clusters. Simulations further showed evidence of the formation of both ½ 111 and 100 interstitial type dislocation loops, as well as the occurrence of cascade collapse resulting in 100 vacancy-type dislocation loops, in excellent agreement with experimental observations. The fractal nature of the cascades gives rise to a scale-less power-law–type size distribution of defect clusters.

The choice of the cut-off energy T_c for electronic stopping was found to have a clear effect on defect clustering. A low cut-off of 1 eV inhibited the formation of large defect structures, whereas $T_c \geq 5$ eV resulted in the occasional formation of large self-interstitial atoms (SIA) and vacancy clusters.

The W work relates to the dpa work in that it shows the possibility to use power laws to predict the distribution of damage in clusters. It also shows that the way the electronic stopping power is treated gives rise to a minor additional uncertainty in predicting the primary damage state accurately.

3. IAEA CRP workplan

Within the IAEA CRP we will collect and critically evaluate MD and experimental data on damage production at least for the metals in Fe, Ni, Cu, Ag, Pd, Pt, W. We will fit the data, including the uncertainty of the data if possible, using a least-squares Levenberg-Marquardt fitting algorithm. The fits will provide element-specific fit parameters b_{arcdpa}^{Fe}, c_{arcdpa}^{Fe}, … including their statistical uncertainties to the data. The fits will be done to composite data for several different interatomic potentials, and as such the uncertainties of the parameters will also include an estimate of the systematic error with respect to the variation of the potentials.

We will also fit the parameters of the new rpa equation for the best existing data on ion beam mixing (= lattice atom replacements) in at least Fe, Ni, Pd, Pt. The fits will provide the parameters b_{mix}, c_{mix} including their statistical uncertainties. The fitting results will also be validated by comparison to experimental data on ion beam mixing coefficients by using a recoil spectrum calculated with the MDRANGE code for specific irradiation conditions for which mixing has been measured in these materials.

In a separate activity, we will simulate the damage production by a combined MDRANGE calculation of recoils spectra and MD full cascade production results in Cu for irradiation conditions matching exactly those at new 4 K experiments to be done by (as part of this CRP activity) by Y. Iwamoto at the Kyoto University facility. We will compare the MD results on total Frenkel pair production with the results on resistivity recovery done in this experiment.

As a closely related activity, we will also carry out this step by using the MDRANGE calculation in connection with the arc-dpa equation to calculate the damage production for the same experiments. This will provide a test of whether the arc-dpa approach gives reliable description of damage production, at least in this relatively simple test case.

Independently of the Fe activities, we will also simulate cascades in bulk quartz as function of energy to enable calibration of the BCA code of CRP participants F. Mota, C.J. Ortiz and R. Vila at CIEMAT. The simulations will be carried out in alpha-quartz using the Watanabe potential for SiO_2, previously found to give good agreement with experimental data for swift heavy ion damage production in SiO_2. We will provide point defect production, analyzed using Voronoy polyhedra, including the statistical uncertainties as a function of energy.

The SPECTER Computer Code for Radiation Damage Calculations

L.R. Greenwood

Pacific Northwest National Laboratory,
P.O. Box 999, Richland, WA
United States of America

The SPECTER computer code [1] was developed to calculate dpa (displacements per atom) and primary knock-on (PKA) energy distributions for 40 different elements and some compound materials. The code is based on the DISCS computer code [2] which calculates the PKA distributions using basic formulas for the nuclear reaction kinematics and neutron cross sections from ENDF/B-V. This version of ENDF did not contain recoil spectra that are now available in later versions of ENDF. The total damage energy is calculated from the nuclear stopping power of the PKA distributions using the Lindhard [3] model for the energy partition between electronic and nuclear stopping. Secondary displacements are determined using the NRT (Norgett, Robinson, Torrens) [4] model. The software contains extensive libraries of the PKA energy distributions as a function of neutron energy and recoil

energy, dpa cross sections for many elements and compounds, neutron cross sections, gas production cross sections, total KERMA, and dpa cross sections for selected compounds as well a few more advanced models of radiation damage. The user of the code only needs to supply the neutron spectrum of interest and length of irradiation time. SPECTER will then provide spectral-averaged values for all of the quantities listed above and as selected for output by the user. No access is required to ENDF or other nuclear data libraries. The code can be executed quickly on any personal computer.

The dpa concept was developed as a way of comparing irradiation effects in materials that were irradiated in very different neutron spectra or ion beam experiments. In such cases, no correlation is possible simply using the particle fluence since radiation damage effects are very sensitive to the significant difference in primary damage energy produced by the spectral differences. The dpa unit was conceived as a way of accounting for such differences in damage energy and it has proven to be quite effective in correlating materials effects data for different neutron environments. One of the earliest examples of such correlation of yield stress in stainless steel is shown in Figure 1 using data from reference 5. The left figure shows yield stress in stainless steel plotted as a function of the neutron fluence above 0.1 MeV for irradiations in the Omega West Reactor at Los Alamos National Laboratory, the 14-MeV Rotating Target Neutron Source II at Lawrence Livermore National Laboratory, and the spallation neutron source at the Los Alamos Radiation Effects Facility. Whereas these data show no correlation with neutron fluence, they show very good correlation with the dpa exposure unit, as shown on the right side of the figure. Such correlations have been seen in many other cases, thus explaining why the dpa unit was adopted for an exposure unit that is not dependent on the neutron spectrum or ion beam energy. Such correlations are especially useful for the study of fusion reactor materials since it allows us to simulate fusion environments, which of course do not yet exist, in other types of irradiation facilities. In the fusion case, the helium/dpa ratio is particularly important due to the high gas production from 14 MeV neutrons in a fusion reactor spectrum.

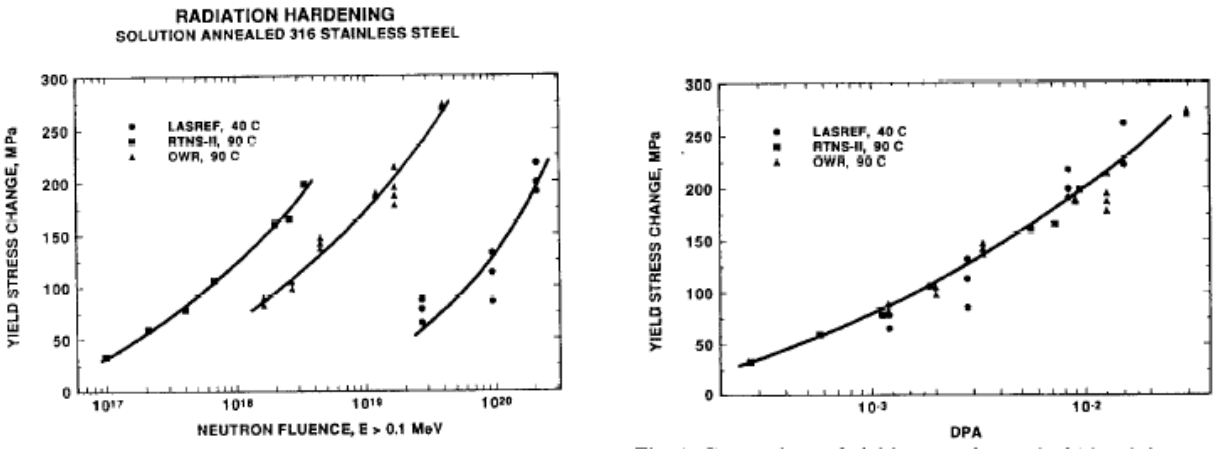

Figure 1. Comparison of yield stress change in 316 stainless steel following irradiation in three radically different facilities, the Omega West Reactor (OWR) at LANL, the 14 MeV neutron source Rotating Target Neutron Source at LLNL, and the spallation neutron source Los Alamos Radiation Effects Facility at LANL. Note the good correlation with dpa, demonstrating the usefulness of this concept.

Capture gamma neutron damage in SPECTER was determined by summing over all of the gamma cascades using relativistic kinematics to determine the net recoil energy. Whereas a single high energy gamma can impart significant recoil energy to the final atom, a cascade of gammas is much less effective since gammas are emitted in various directions according to known angular distributions. The average recoil energy is thus calculated and used to determine the net damage energy. Since the final nucleus also frequently rapidly undergoes beta decay following neutron capture, this decay significantly contributes to the total damage energy. Beta decay should thus be included in future

calculations of neutron capture displacement damage, but is typically neglected. The end point beta energy and type of beta decay can be used to determine the average recoil energy.

SPECTER calculates both the differential and integral PKA energy distributions averaged over the input neutron spectrum. Values are provided both with and without reference to the displacement energy. The integral of the differential PKA spectra are equal to the total nuclear interaction cross section. However, in many cases involving significant thermal or epithermal neutrons, many of the PKA have very low recoil energies. Consequently, SPECTER provides the PKA spectra without considering the energy that is required to produce a recoil and also the PKA spectra that has energies above the threshold since lower energy events do not have the required energy to create a Frenkel pair in the NRT model.

Figure 2 shows the calculated PKA spectra for each type of nuclear reaction as well as the total PKA spectrum for nickel irradiated in the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory on the left side. The right side compares integral PKA spectra for many different irradiation facilities including HFIR, a typical fusion reactor first wall spectrum, the Fast Flux Test Facility (FFTF) at PNNL, the spallation source Intense Pulsed Neutron Source at Argonne National Laboratory, a ^{235}U fission spectrum, and a 14 MeV neutron spectrum.

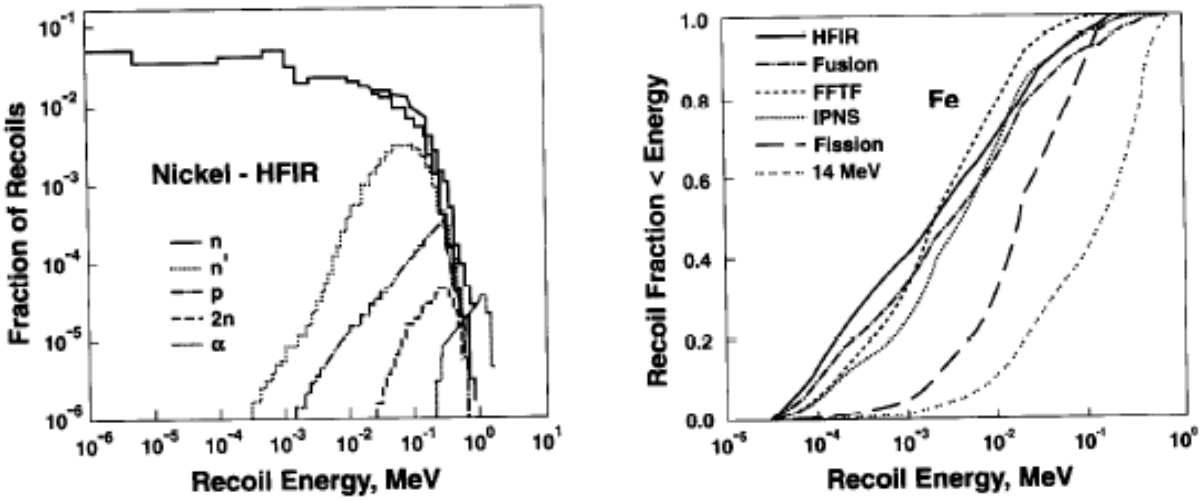

Figure 2. PKA spectra calculated by SPECTER are shown for the HFIR reactor at ORNL (left) and integral PKA spectra for a variety of neutron irradiation facilities (right).

The SPECOMP [6] computer code was developed to calculate radiation damage in compound materials. Any combination of five elements may be specified. The main problem with doing such calculations is the determination of the correct displacement energies to use since they are not the same as for pure elements. In some cases molecular dynamics calculations provided these values such that calculations could be done. The results were added to SPECTER such that the dpa are calculated for these compounds whenever SPECTER is executed. The SPECOMP program was further used to calculate more advanced damage functions such as freely migrating defects and cascade formation [7].

Figure 3 shows an example of the displacement cross sections calculated for Li_2O showing the contribution from each combination of recoil ion and matrix atom as a function of neutron energy.

SPECTER has been widely used to calculate dpa, gas production and KERMA for many years in order to characterize neutron irradiation experiments and to provide a basis for correlation of materials irradiation effects between widely diverse neutron spectra. The main limitation is that the cross sections were derived from ENDF/B-V and should be updated with newer cross section information. Other limitations that are usually common to newer codes are that nuclear burn-up and transmutation effects (other than gas production) are not included and may become very important at higher neutron fluencies. The cross sections also need to be extended beyond 20 MeV for use with accelerator-based neutron sources.

Both the SPECTER and SPECOMP codes are available on the NDS/IAEA web-site https://www-nds.iaea.org/irdf2002/codes/index.htmlx .

One very important consideration in updating dpa cross sections is that there is a very large database of materials effects in the literature that has used dpa as an exposure parameter. The ASTM has recommended the use of standard radiation damage cross sections so that such data are all provided on the same basis, such as ASTM E693. If we update dpa cross sections with every revision of nuclear data, then care must be taken to preserve the relationship with prior data that exists in the literature including radiation materials handbooks and regulatory guides.

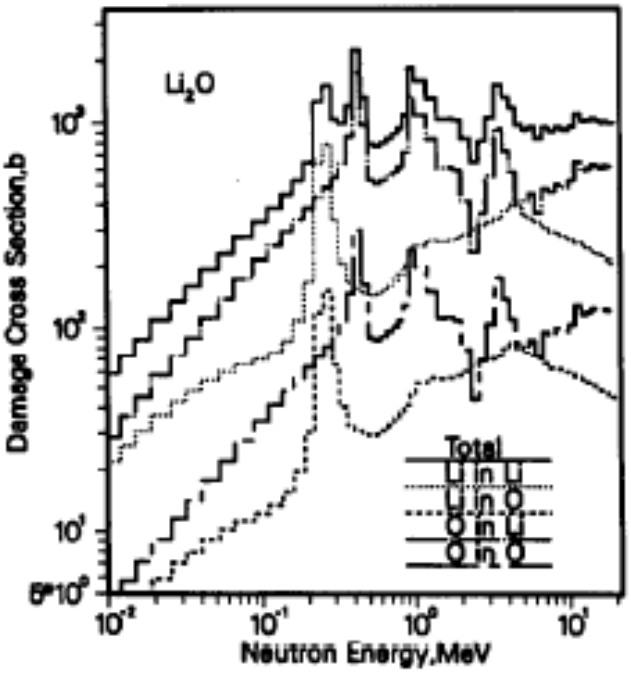

Figure 3. Displacement damage cross sections calculated with SPECOMP for Li_2O.

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Evaluation of displacement and gas production cross-sections for structure materials using advanced simulation methods and experimental data

A.Yu. Konobeyev, U. Fischer

Karlsruhe Institute of Technology
Karlsruhe
Germany

The objective of the report is to review briefly problems and solutions concerning the evaluation of displacement and gas production cross-sections at intermediate energies of primary particles and to discuss the tasks planned to be performed in the frame of the CRP.

The calculation of displacement cross-sections consists of two independent parts: the calculation of recoil energy distributions in nuclear reactions and the number of stable displacements in materials. The evaluation of gas production cross-sections supposes the estimation of different components of hydrogen and helium production cross-sections. Calculations show that a main contribution to hydrogen and helium production is due to the proton and α-particle emission, at the same time the contributions of deuterons, tritons, and ^{3}He are important enough to be considered by the cross-section evaluation. For example, the deuteron emission makes up 15 % of hydrogen production depending on a target and primary particle energy.

It is planned to perform cross-section evaluations up to 3 GeV taking into account important applications of evaluated data for spallation neutron sources and other advanced facilities. A low energy limit is defined for incident neutrons by the corresponding energy employed in nuclear data libraries, and for incident protons by a threshold displacement energy E_d. The radiation damage rate for structural materials in reactors is most sensitive to the displacement cross-section at neutron energies above 10 keV; for incident protons the energies of interest are above 0.5 keV.

1. Comparative analyses of the information available in the nuclear data libraries used for the calculation of recoil energy distributions. Assessment of the uncertainties associated with the use of data from different sources and nuclear models

Important questions to be answered here are:

- are recoil energy distributions calculated using data from different sources in agreement?
- should one choose “the most reliable” data library or use a statistical weighted sum using data from various data files for final evaluation of displacement cross-section?
- are the $d\sigma/dT$ values from the libraries in agreement with calculations using intranuclear cascade evaporation models (MCNPX) at incident energies above 20 MeV?
- can one rely on approximate calculations performed by deterministic codes?
- what is the impact of uncertainty of $d\sigma/dT$ values on calculated displacement cross sections?
- what is the error of evaluated displacement cross-sections taking into account an uncertainty of $d\sigma/dT$ values and of the number of stable defects produced in materials?

Preliminary calculations show a rather large difference between recoil energy distributions obtained using data from ENDF/B-VII-0, ENDF/B-VII.1, JEFF-3.1.2, TENDL-2011, and results of calculations using intranuclear cascade evaporation model. Figures 1 and 2 show typical $d\sigma/dT$ values obtained. NJOY [1] and SPKA [2] codes were used to get recoil energy distributions from libraries.

The study of uncertainties of displacement cross-sections associated with $d\sigma/dT$ values obtained from different sources should include the information from ENDF/B-VII.1, JENDL-4, and up-to-date versions of JEFF and TENDL libraries.

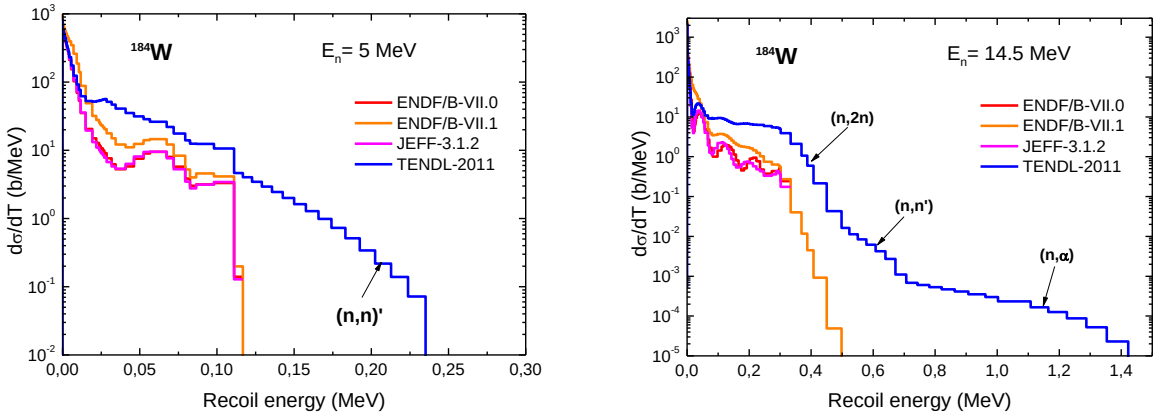

Fig. 1. Total recoil energy distributions resulting from elastic and nonelastic interactions of neutrons with ^{184}W at the incident neutron energy 5 and 14.5 MeV calculated using data from different nuclear data libraries.

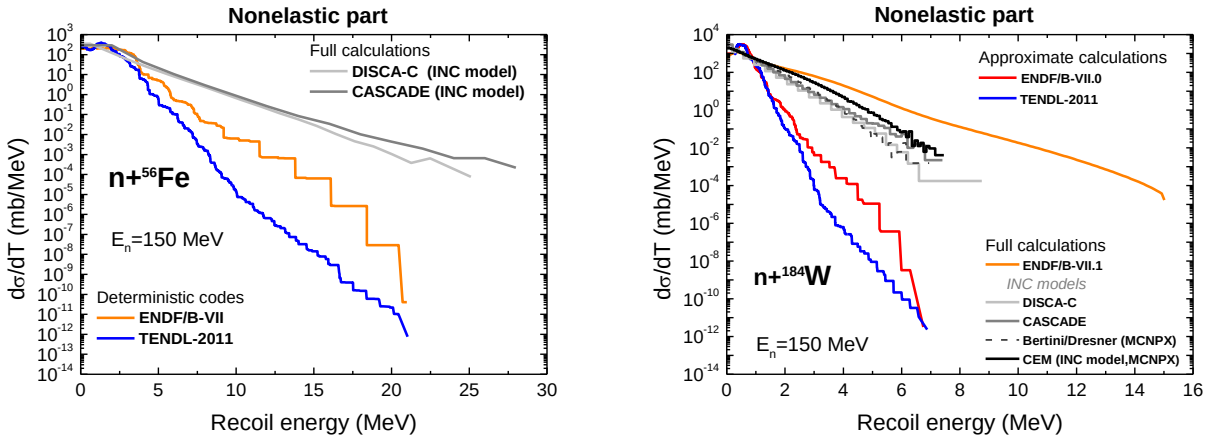

Fig. 2. Recoil energy distributions for nonelastic neutron interactions with ^{56}Fe and ^{184}W at the incident neutron energy 150 MeV calculated using data from different nuclear data libraries and using intranuclear cascade evaporation models.

2. Calculation of displacement cross-sections for important structural materials using latest results of molecular dynamics simulations. Modeling of defect production in materials using the binary collision approximation model with corrections based on results of molecular dynamics simulations

Concerning the application of nuclear models the calculation of displacement cross-section σ_d consists of two rather independent parts: the calculation of σ_d for elastic scattering of primary particles on atoms and for nonelastic particle interactions with nuclei. Each part of the calculation is associated with a specific uncertainty resulting from the use of appropriate nuclear models and sets of model parameters. The additional uncertainty of σ_d originates from the evaluation of the number of stable displacements in irradiated material.

The proposed method for the calculation of the number of stable defects in materials consists of the following steps:

- simulation of interactions of primary particles with a target nuclei using the intranuclear cascade evaporation model
- modeling of collision cascades in the material for ions (Z_i,A_i,T_i) produced after the nuclear reaction using the binary collision approximation model [3] up to a certain "critical" kinetic energy of ions T_{crit}

- calculation of the number of stable displacements based on results of molecular dynamics simulation for ions with energies below T_{crit}.

The modeling of nuclear interactions at energies above several tens of MeV is performed using different versions of the intranuclear cascade evaporation model implemented in the MCNPX code [4] and the CASCADE (JINR, KIT) code [5]. A difference of the results of final σ_d values can be attributed to the uncertainty of evaluated displacement cross-sections associated with the use of nuclear models.

Fig. 3 shows typical differences of σ_d values obtained using various versions of intranuclear cascade evaporation model.

Previously, displacement cross-sections were calculated for a number of materials [6] using the approach discussed above. It is planned to perform the new evaluation of σ_d values for other materials important for applications and for materials from Ref. [6] using new results of MD simulations, if available.

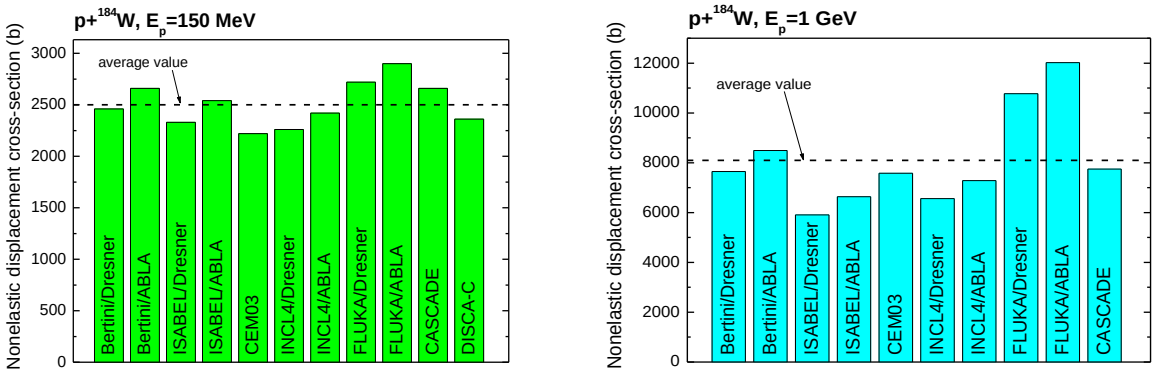

Fig. 3. Examples of displacement cross-sections corresponding to nonelastic interactions of protons with ^{184}W calculated using different codes utilizing the intranuclear cascade evaporation model. The number of defects is calculated according to the NRT model.

3. Evaluation of gas production cross-section and its components: proton-, deuteron-, triton-, ^{3}He-, and ^{4}He- production cross-section for structural materials at primary nucleon energies up to several GeV using advanced nuclear models and available experimental data

The main problem concerning the use of experimental production cross-sections of hydrogen and helium isotopes for the data evaluation are:

- A large scatter of the data obtained by different authors
- Lack of the description of details of the measurements complicating an analysis and a possible correction of the data
- Measurements of the yields of H-, and He- isotopes with energies making a part of a whole energy range of the emission.

Before the use of EXFOR data results of measurements should be analyzed and corrected, if necessary.

The main problem of model calculations of gas production cross-sections at intermediate energies is the modeling of non-equilibrium emission of light clusters. With varying degrees of success, the problem was solved in new versions of programs ALICE/ASH [7], CASCADE [5], TALYS [8], and MCNPX [4].

It is planned to perform the evaluation of hydrogen and helium production cross-sections for materials of interest in an addition to evaluated data [6]. Examples of evaluated cross-sections are given in Fig.4.

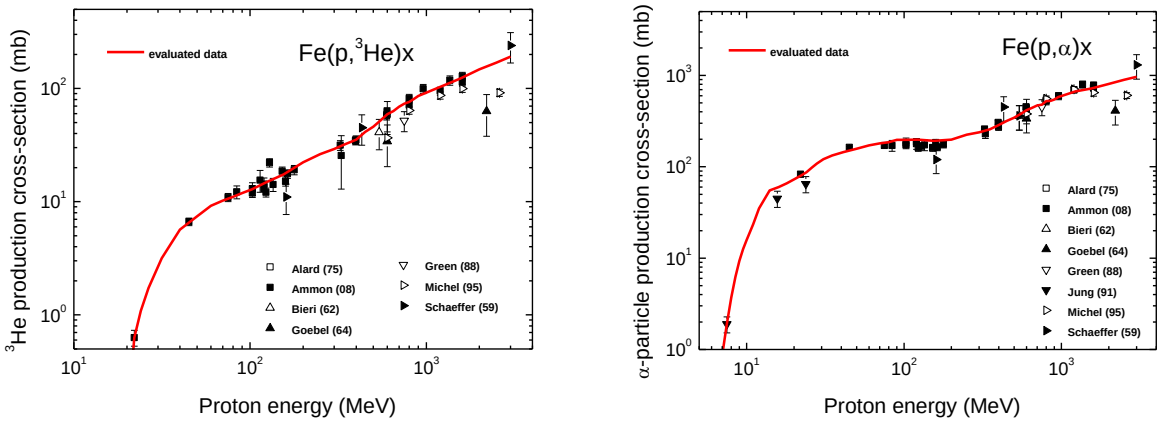

Fig. 4. Examples of evaluated ^{3}He- and ^{4}He- production cross-section for proton induced reactions with iron.

4. Conclusion

The main goals of the planned work are the analysis of uncertainties of calculated displacement cross-sections associated with the calculation of recoil energy distributions in nuclear reactions and the evaluation of displacement and gas production cross-sections for structural materials using results of advanced model calculations and experimental data.

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Calculation of PKA and DPA using event generator in PHITS code

Yosuke Iwamoto and Tokio Fukahori

Japan Atomic Energy Agency
Shirakata-Shirane 2-4, Tokai, Ibaraki, 319-1195
Japan

Our researches relevant to CRP:

To implement the DPA calculation method in the particle and heavy ion transport code system (PHITS) [1], we have developed a method that allows calculating the DPA and PKA values using the event generator in PHITS. The procedure for the calculation of the DPA value is as follows [2].

(1) The kinetic energies of PKA or secondary charged particles, including residual nuclei, are determined using intra-nuclear cascade evaporation models in high energy region. In addition, the event generator mode for low-energy neutron irradiations is also used to estimate PKA energies. In this mode, the evaluated nuclear data for neutrons and a special evaporation model are combined so as to trace all correlations of ejectiles keeping the energy and the momentum conservation in a collision.
(2) The damage energy, which characterizes the displacement cascade, is then derived from these energies, considering the ratio of energy losses due to the elastic scattering of lattice atoms and the electronic excitation.
(3) The displacement cross-section between PKA or the secondary charged particle and the target atom is calculated from the damage energy in each event, using the Norgertt-Robinson-Torrens (NRT) model, which predicts only the number of initially displaced atoms produced in the cascades of atom-atom collisions, and the universal one-parameter differential Coulomb scattering cross-section.

Displacement cross-section is calculated with Coulomb scattering using the following equation:

$$\sigma = \int_{td}^{tmax} \frac{d\sigma_{sc}}{dt} \eta N_{NRT} dt \qquad (1)$$

where N_{NRT} is the number of defects produced in irradiated material, σ_{sc} is a universal one-parameter differential scattering cross-section equation in reduced notation, η is the defect production efficiency (number of survived defects to NRT predictions) [3].

Figure 1 shows calculated results of DPA values using PHITS and FLUKA codes for the 800 MeV protons incidences on a 5 cm radius × 40 cm length copper target. PHITS and FLUKA results agree within a factor of two. In higher energy, nuclear reactions occur before the stopping range is reached and DPA values created by secondary particles are increased with energy. For 800 MeV, well-developed hadronic cascades are appeared. In general, for the neutron and proton beams in the energy range from 10 MeV to 1 GeV, the calculated results of PHITS agree with those of other Monte Carlo codes such as FLUKA and MARS codes within a factor of two.

Figure 2 shows the comparison between the $\sigma_{BCA\text{-}MD}$ that was calculated using the PHITS and the data that was taken from the KIT data file [4] that included the displacement cross-sections for iron and copper that were irradiated with protons and neutrons [5]. For the irradiation with protons, the PHITS results are in a good agreement with the KIT data over a wide range of energies. For the irradiation with neutrons, the agreement between the two sets of results is also satisfactory. Note that the neutron resonance cross-section for the PHITS results disagrees with the KIT data because of the different meshes of neutron energy.

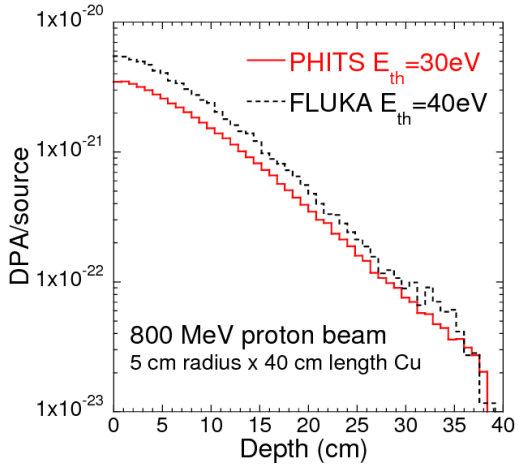

Fig. 1. Calculated results of DPA values using PHITS and FLUKA codes for the 800 MeV protons incidences on a 5 cm radius × 40 cm length copper target.

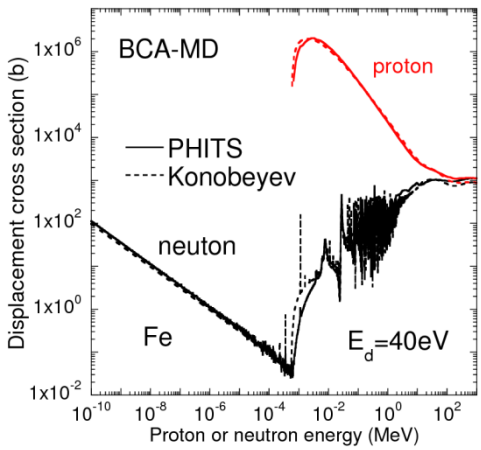

Fig. 2. Comparison between the $\sigma_{BCA\text{-}MD}$ that was calculated using the PHITS and the data that was taken from the KIT data file.

Our activity related to CRP

Although we developed the calculation methods of PKA and DPA values in PHITS code and compared with several methods, intercomparison of calculation methods is not sufficient. Furthermore, we do not know how PKA spectra affect DPA values. Therefore, to clarify the problem of PKA spectra related to displacement cross sections, systematic intercomparison of various calculation methods of PKA spectra and displacement cross sections is needed.

In the first two years, we will calculate PKA spectra and displacement cross sections in the same calculation condition using various models such as PHITS event generator and ESPERANT using nuclear data libraries for neutron and proton incidences. EPERANT code is processed from Neutron Data in the JENDL High Energy File up to 50 MeV by using Effective Single Particle Emission Approximation (ESPEA) [6]. After the intercomparison of methods, we will find the difference of results between methods and point out the problem.

Another activity is measurement of displacement cross sections using the electrical resistance measurement method for 150 MeV proton on Cu wire target at around 4°K at the FFAG accelerator facility in Kyoto university research reactor within first two years. This experiment will provide data to assess codes that are used to predict the displacement cross sections and the primary radiation damage. If this experiment is successful within two years, measurements of electrical resistance on Al and Fe will also be done in third and fourth years.

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Uncertainty Analysis of Metrics Used for Assessing Primary Radiation Damage

P. Griffin

Sandia National Laboratories
P.O. Box 5820 Albuquerque NM 87185
USA

Sandia has a strong interest in the modeling, validation, and uncertainty quantification of the primary neutron displacement damage to electronics, in particular in the gain degradation of minority carrier devices such as bipolar transistors. Resistivity experiments in bulk silicon have shown a good correlation of the change in resistivity and the neutron displacement kerma received in a radiation exposure. The same good correlation is observed in the change in the reciprocal gain in bipolar transistors. This gain degradation is related to the change in the minority carrier lifetime caused by the neutron-induced defects, and comes from the same source of degradation as is affected the bulk resistivity measurements. In fact there is an ASTM standard, E1855, that uses the gain degradation in a 2N2222A npn transistor as a dosimeter for neutron irradiations. Time/temperature annealing of the neutron-introduced defects can alter the transistor gain degradation, so the standard calls for use of a temperature-stabilized gain degradation measurement. For cases where there is charged particle equilibrium, the neutron displacement kerma is identical to the neutron displacement dose, or what is often just referred to by the material damage community as the neutron damage energy.

The gain degradation in GaAs devices, such as heterojunction bipolar transistors (HBTs) and LEDs are also related to the introduction of electrically active defects that charge the minority carrier lifetime. In the case of GaAs, experiments with DT, DD, fast fission, and water-moderated fission neutron spectra have shown that the gain degradation is altered from that predicted by a straight dependence on the displacement kerma by a factor that can be related to the energy of the primary recoil atoms – more clustered damage exhibiting a reduced number of residual electrically active defects. Other semiconductor materials of interest to the radiation effects community include InP, SiC, GaN, and Ge.

We propose, in the first year of this CRP, to:

1. Revisit and summarize the experimental data underlying this damage correlation for semiconductor materials with the neutron displacement energy.
2. Examine what can be deduced concerning the energy-dependent covariance for the neutron displacement kerma in silicon and determine how this uncertainty information should be applied to the use silicon displacement damage monitors and to the validation of the correlation of the neutron displacement kerma with the reciprocal change in the gain of bipolar transistors.

In support of objective 2 above, we propose to:

- Use a random sampling of the TENDL-2013 ^{28}Si cross sections and a Total Monte Carlo approach to obtain a covariance matrix for the TENDL-2013 ^{28}Si neutron displacement kerma.
- Examine the importance of the Total Monte Carlo approach to this application by investigating the role of cross-reaction correlations in the covariance for the total cross section and for the neutron displacement kerma.
- Through a comparison of the covariance of the total cross section and of the displacement kerma, determine the importance of the uncertainty in the recoil spectra to both the energy-dependent uncertainty and to the shape of the correlation matrix.
- Investigate the consistency of various sources of information regarding the PKA recoil atom spectra for various reaction channels in ^{28}Si and determine if this supports the observations from the preceding bulleted item.
- Investigate the importance and role of various uncertainty contributors related to the damage partition function to the neutron displacement kerma.
- Highlight any energy regions where “model defect” may have yielded, through the Total Monte Carlo approach, a smaller uncertainty than is consistent with the spread seen in experimental measurements.
- Since silicon electronics are composed of ^{nat}Si rather than isotopically pure ^{28}Si, address the importance of including the other silicon isotopes in calculating the neutron displacement kerma

for actual devices. Place this consideration of silicon isotopes in context with the importance of modeling the device dopants, typically boron in n-type regions and phosphorus in p-type regions, while calculating the displacement kerma.

- Make proposals for how the electronics damage community should apply an quantified uncertainty estimates that may be obtained through the Total Monte Carlo application of the TENDL-2013 cross section sampling.

Calculation of the damage energy in polyatomic materials using nuclear cross section evaluations

L. Luneville, J.P. Crocombette, D. Simeone

French Atomic Nuclear Agency, CEA Saclay Centre
France

When a material is subjected to a flux of high-energy particles, its constituent atoms can be knocked from their equilibrium positions with a wide range of energies, depending on the exact nature of the collision. The spectrum of damage energy, derived from the exact knowledge of the recoil spectra for each nuclear reaction occurring in the solid, constitutes a vital data set required for understanding how materials evolve under irradiation**.** The project will be aimed at using the latest, most modern nuclear data to produce, evaluate and assess the damage energy spectra for a range of nuclear-relevant materials. The knowledge of such a damage energy is relevant to compare the impact of different facilities on the structural behaviour and relevant properties of materials.

I-1. Calculation of the damage energy

In order to describe primary damage produced in materials, our group has already developed an estimation of the damage energy via the DART code [1] for mono atomic and polyatomic materials. This code exhibits three interesting features in comparison with previous similar codes:

- Since nuclear reaction is associated to isotopes and not to elements forming material, the DART code has been specifically design to handle recoil spectra on each isotope. Thanks to this code, it is then possible to extract not the average value of the recoil energy of recoils for an element but the exact energy of recoils associated with the different isotopes of a defined element.
- On the other hand, DART allows to take into account the angular anisotropy (with a set of Legendre polynomial) of recoils
- In this approach based on the Binary collision Approximation framework, it is possible to estimate the damage energy induced by recoils and fission products materials using the general partition of the energy derived from the Lindhard formalism and not from the Robinson and NRT formalism. The interest of such an analysis is due to the fact that the elastic energy given by a light particle (helium, proton) in a heavy matrix can be safely determined.

As an example of application of the DART code, Figure 1 displays the impact of the angular anisotropy on the total energy damage cross section.

I-2. The proposed research in the CRP

Within the research project, it is intend to examine the recoil Primary Knock on Atom (PKA) energy spectra in the TENDL-2012 and ENDF/B-VII.1 nuclear data libraries and derive from them the damage energy (or atom displacement) cross sections for the nuclei of materials of interest. Above the two particles emission threshold, the current nuclear reaction modelling of the PKA spectra, essentially dependent on approximations used, appears too simplistic and the development of higher quality more accurate treatment is required. Additionally, in the high neutron-energy range the processes involving the recoil of secondary energetic (light) particle nuclei and the (heavy) residual makes significant contribution to the damage, hence more accurate evaluation of their energies and reaction cross-sections is needed.

For this reason, the proposed research presented in this work involves tight and sequential collaboration efforts with both, the Nuclear Research and Consultancy Group NRG, Petten, the Netherland and the CCFE/Fusion at Culham.

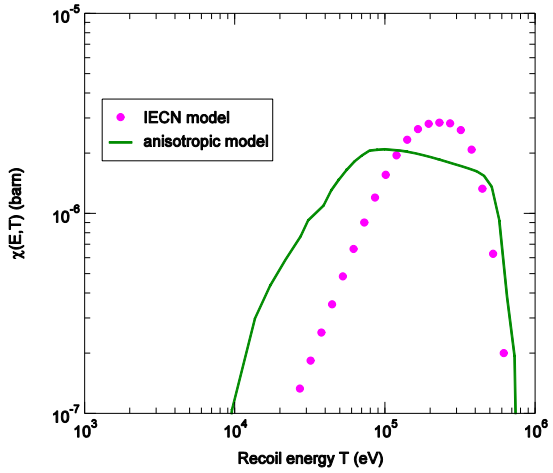

Fig. 1a. Recoil cross section on ^{56}Fe induced by 14 MeV monokinetic neutrons derived from the anisotropic model (DART: green lined) and determined for the evaporation model (Isotropic Evaporation Compound Nucleus: pink dots)

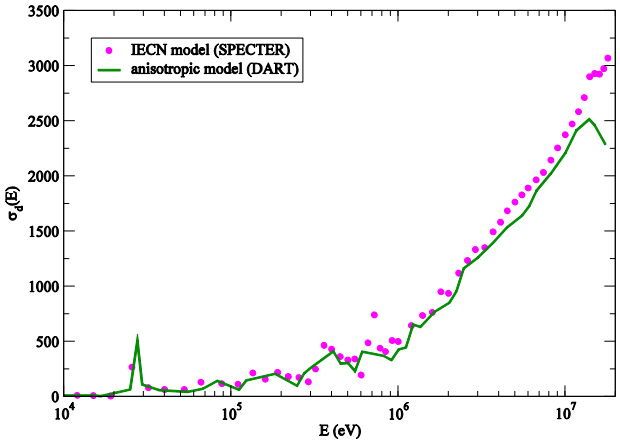

Fig. 1b. Impact of the anisotropy (green line) of the damage energy cross section. For neutron with kinetic energy above 1 MeV, a large discrepancy is observed.

Figure 2 displays first results resulting from this collaboration. A comparison of damage energy cross section on ^{56}Fe versus the neutron energy calculated with the DART code using ENDF/B-VI and TENDL-2012 data.

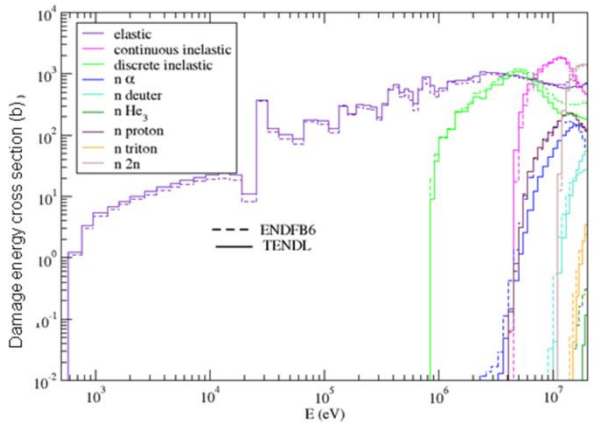

Fig. 2a. Calculation of the damage energy cross section versus the neutron energy on ^{56}Fe atoms with the DART code using both ENDFB-VI (dashed line) and TENDL-2012 (full line).

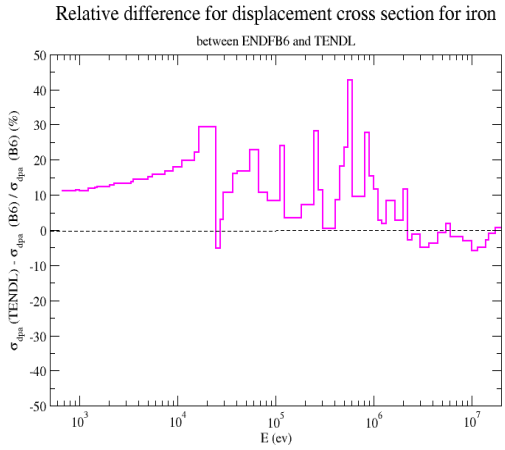

Fig. 2b. Relative errors associated with the use of two distinct libraries for neutron energy below 14 MeV.

II-1. Translation to defects induced by irradiation in materials

The approach developed in the DART code remains nevertheless unsatisfactory. The damage function is far from being a faithful description of defects (point defect, dislocation loops, voids) produced by irradiation in solids. Only the Molecular Dynamics technique is able to mimic radiation damage in material. We want, using this technique, to focus on the applicability of the laws measuring the

amount of damage (NRT dpa and beyond) to multicomponents solids. Indeed the NRT-dpa formula has been designed for single element solids, especially pure metals. It is sometimes applied to alloys or compounds without solid theoretical grounds, with a threshold energy value obtained with some kind of averaging. The recently proposed new formulas for damage production are also primarily designed for mono-elemental solids.

II-2. The proposed research in the CRP

We propose first a reassessment of Molecular Dynamics (MD) calculations available in literature or performed in our laboratory, complemented if needed by dedicated additional calculations.

On one hand a bibliography study shall be performed on ordered metallic or ionic compounds to obtain data on surviving Frenkel pairs and replacements per atoms. The results of this search shall allow a first checking of the damage formulas.

On another hand, for what concerns our own MD works, we shall focus on ZrC [2] and UO_2 [3].

First, we should consider the case of ZrC ceramic. In this material cascades resulting in point defects and very small dislocation loops have been observed. Moreover sub-cascades seem observable. We shall try to measure in details the number of replaced atoms and surviving Frenkel pairs on each sublattice. In order to do so new simulations of high energy cascades (50 -100 keV) are needed.

Second, in spite of its structural simplicity and its damage simply made of point defects, UO_2 is an interesting case. First it is obviously an important nuclear material. Second series of MD cascade simulations at increasing PKA energies show a continuous decrease of the amount of created point defects compared to the NRT formula. This means that the saturation of the decrease of the efficiency factor has never been observed by MD cascade simulations. Moreover Pseudo Binary Collision Approximations (BCA) calculations show that the division in subcascades seems not to take place in this material. We plan to perform MD cascades of large energy PKAs to try to observe sub-cascade formations. The OECD-NEA formula being based on this subdivision, its applicability for UO_2 is not guaranteed.

Based on all these data we shall try to see if the efficiency factor is equal for all sublattices. In this case they would only differ by their respective displacement energies. More probably we shall have to define distinct efficiency for each sublattice. The applicability of the new formulas shall then be checked and if they apply the relations between the parameters for each sublattice shall be identified.

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dpa and beyond: recoil spectra and physical damage indices

J.-Ch. Sublet and M.R. Gilbert

United Kingdom Atomic Energy Authority, Culham Science Centre
Abingdon, Oxfordshire, OX14 3BD
UK

The concept of dpa, whether NRT or otherwise, is limited in its ability to describe radiation damage. In particular, it does not properly account for the evolution of defects. A complete picture must, desirably, include simulation and modelling of the time evolution in defect structures and populations.

Computational simulations, such as atomistics with molecular dynamics, can simulate the cascade of damage caused by an initial recoil event (the "primary knock-on atom" or PKA) and track subsequent evolution. With modern computers we are, perhaps, reaching a point where it will soon be possible to build up a statistical picture of defect evolution as a function of PKA energy. In this case, a more useful direct link between simulation of the neutron irradiation environment and atomistic simulation is a complete picture of the population of PKAs as a function of energy – so-called recoil spectra.

As a part of the United Kingdom Atomic Energy Authority's contribution to the CRP, we will use the latest techniques to evaluate up-to-date nuclear data to develop a consistent and robust methodology to produce the complete set of recoil spectra, including the correct differentiation as function of recoiling species, for a given material, whether a single isotope or complex alloy, in a given neutron irradiation field. Additionally, the latest version of the inventory package EASY-II [1] can calculate the time evolution in NRT dpa/year and other damage indices for the complete inventory of nuclides, as well as gas production rates using in-built cross section libraries processed through NJOY. Uniquely, the full energy dependence of each quantity is properly taken into account. For example, the Figure 1 below shows the cross sections for various gaseous species from ^{90}Zr, along with the partial displacement cross sections for ^{184}W. The high computational efficiency inherent to the current FISPACT-II [2] inventory code in EASY-II [1], together with dedicated libraries [3, 4], will enable rapid comparison, via simple indices like dpa/year values, dpa/He ratios or above 1 MeV fluence, of different irradiation conditions and/or different materials.

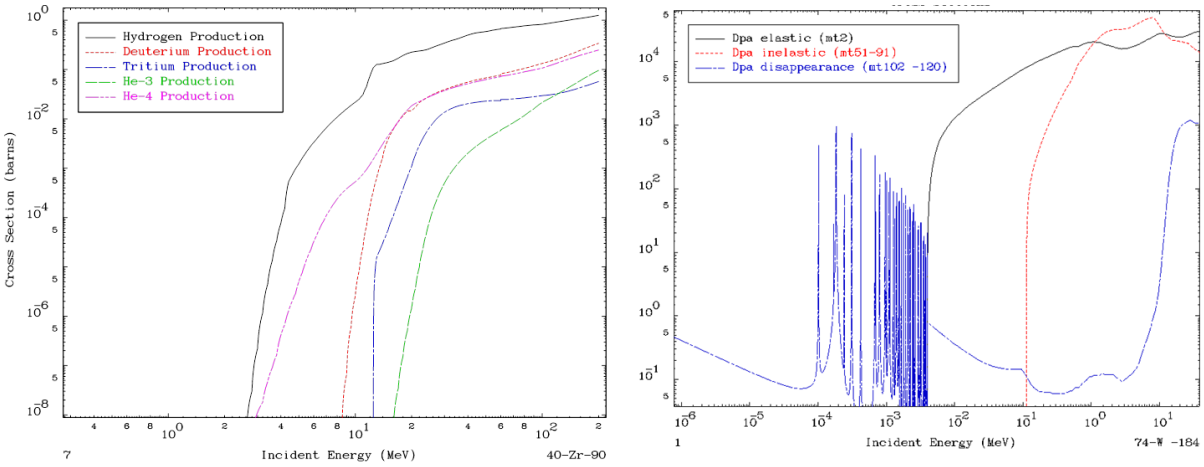

Figure 1. Gas production cross sections on ^{90}Zr, and partial displacement cross sections for ^{184}W.

An example, highlighting these capabilities, is shown below in Fig. 2, where the variation in dpa per full power year in a complex steel alloy is given for the full polodial variation in irradiation conditions in the FW armour of four different concepts for a demonstration fusion power plant. Such large-scale calculations can be done rapidly and repeatedly to perform scoping studies of radiation damage indexes. Our contribution to the CRP will also include the required framework within EASY-II, perhaps including additional exposure indices selected by the community (arc-dpa, damage energy, neutron fluence, decay contributions, etc.), to calculate such damage indices as a function of material and irradiation environment.

Returning to recoil spectra, we have, so far, developed a computational tool to take PKA recoil cross sections, output from NJOY, collapse them with a given neutron irradiation spectrum, and perform the necessary summing as a function of recoiling nuclide or element over a given set of input parent nuclides (for example the four naturally occurring isotopes of Fe, with appropriate weighting). Specifically, as well as the heavy nuclide recoils from a given parent isotope, we also consider the recoiling secondary emitted particles, such as α-particles and protons. Typically, such light particles carry higher energies than the primary recoil heavy nuclide, and travel greater distances within the material before losing this energy.

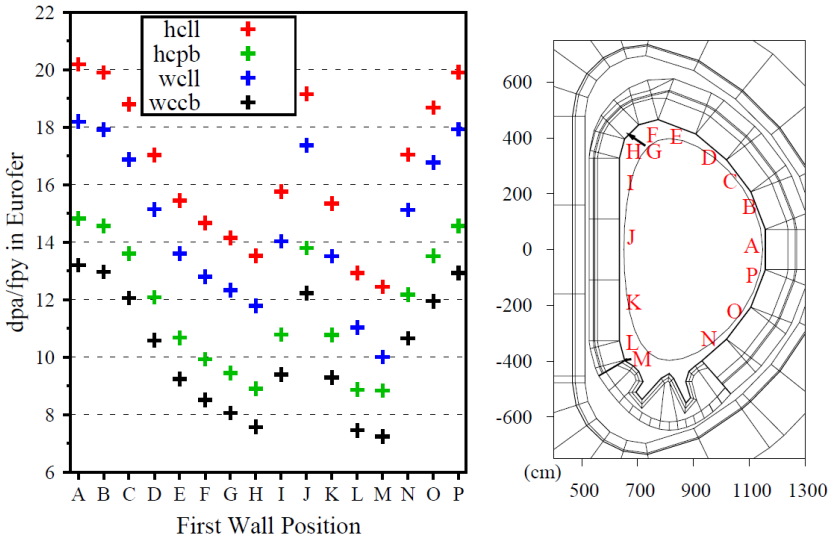

Figure 2. dpa/fpy in Eurofer steel variation with position in FW armour of four DEMO concepts. hcpb is helium-cooled with a ceramic pebble-bed tritium-breeding blanket of Be+Li and wccb is the equivalent water-cooled concept. hcll is helium-cooled with a liquid lithium-lead breeder and wcll is the water-cooled version.

This "proof of principle" as demonstrated in the Fig. 3, which shows the set of recoil spectra for the main ^{56}Fe nuclide of Fe under a typical DEMO fusion reactor spectrum, must be carefully checked for robustness and completeness. Once this is complete, the PKA recoil cross sections will be included in EASY-II and eventually it will be possible to produce recoil spectra automatically and routinely as part of inventory calculations.

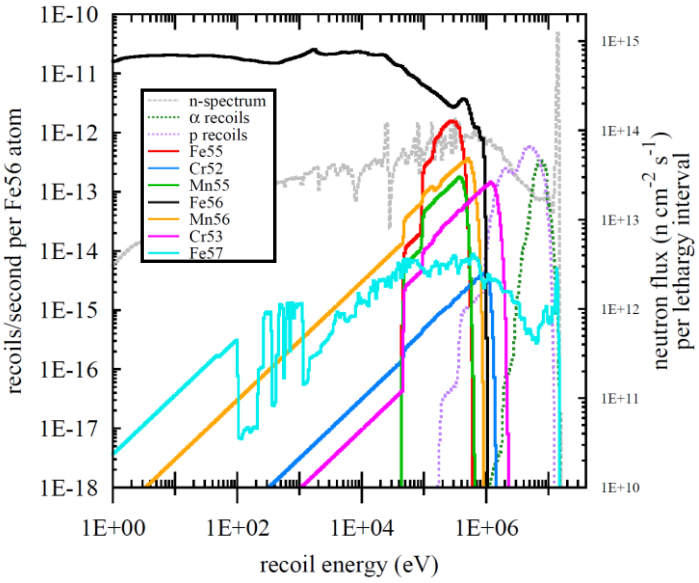

Figure 3. A preliminary set of species dependent recoil spectra for ^{56}Fe under a typical DEMO fusion reactor first wall armour spectrum (also shown on the plot using the right-hand y-axis). The recoil spectra were derived by NJOY using the ENDF/B-VII.1 nuclear data library.

A further goal, within the CRP, is to prepare these properly folded energy dependent recoil spectra for realistic materials (i.e. not single isotopes) for use by CEA to evaluate the damage energy partition function within the BCA approximation using a dedicated program (DART). This collaborative effort should enable us to predict the build-up and of cascade damage in materials subject to neutron irradiation. The impact of burn-up and depletion, where the material composition changes, will also be investigated.

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Evaluation of damage energy cross-section up to 150 MeV and generation of their uncertainty

O. Cabellos

Instituto de Fusión Nuclear
Universidad Politécnica de Madrid
Spain

The aim of this work is to generate a complete neutron damage energy cross-section library up to 150 MeV including uncertainty estimation. Thus, the processed library, in a pointwise or multigroup energy structure, could be used in different nuclear applications. The work is focused on the main structural materials: metals (Al, Ti, V, Cr, Fe, Ni, Cu, Zr …), other metals (Ni, Pt, W ...) and non-metals (Si, Be ...).

Firstly, processing and comparison of damage energy cross-section data from different ENDF files is planned. NJOY99 will be used to perform the processing. The accuracy and completeness of current nuclear data libraries (JEFF-3.1/x, ENDF/B-VII.1/x, TENDL-20xx, …) be assessed for different isotopes or materials. Visualization of these damage energy cross-sections will be performed with JANIS-4.0.

At present, a rough comparison between JEFF-3.1.1 and ENDF/B-VII.1 up to 150 MeV shows:

- Good quality and good agreement between both libraries is found for ^{27}Al, ^{61,62,64}Ni and ^{63,65}Cu.
- An unphysical discontinuity at 20 MeV due to the lack of information of recoil and charge particle distributions above 20 MeV is found for ^{54,56,57,58}Fe in JEFF-3.1.1. This jump is not found in ENDF/B-VII.1
- No information above 20 MeV:
    - JEFF-3.1.1: ^{58,59,60}Ni, Cr, V, Ti and Zr
    - ENDF/B-VII.1: Ag, As, Ba, Be, Ga,Ge, Hf, In, Mo, Sn, Ti, Zn and Zr.
- Some additional problems between 5 MeV to 20 MeV occur:
    - JEFF-3.1.1: ^{54,57,58}Fe, ^{52}Cr and $^{46-50}$Ti, …
    - ENDF/B-VII.1: Ca, ^{55}Mn, W, ^{93}Zr and some isotopes of Pb.

Secondly, an assessment for damage energy cross-sections above 20 MeV is considered. It can be seen that some isotopes in JEFF-3.1.1 (such as ^{54,56,57,58}Fe) show an unphysical discontinuity at 20 MeV. In order to understand the problem at 20 MeV, an update in NJOY to calculate sensitivities to different channel reactions is needed. In particular, the information of neutron production reactions and MT5 section is needed. This sensitivity analysis of the damage energy cross-section to the different nuclear reaction channels of many reactions will be used to understand the problem of this jump.

For instance, it is well known for ^{56}Fe that above 20 MeV only contributions to neutron elastic and MT5 data can be found. So, large differences are expected for MT5 contributions between JEFF-3.1.1 and ENDF/B-VII.1. The reason of this difference is because in JEFF-3.1.1 there is a lack of recoil

information for some important reaction channels, and only H, D, T and He channels are considered. This behaviour of JEFF-3.1.1 is also found in ^{54,57,58}Fe. To solve this problem, a reasonable approximation based on the damage energy cross-section processed with TENDL20xx will be developed.

The third step will be the implementation in NJOY/HEATR of a damage efficiency factor coming from BCA-MD model. Thus, a better agreement with available experimental data comparing with the common NRT formula is expected. The proposal by the OECD/NEA primary damage group proposal [see K. Nordlund et al. in this Report] having an efficiency factor for each material as a function of "b" and "c" parameters will be implemented in NJOY. This parameterization will be as two new parameters in the NJOY input ($\zeta = f(b,c)$).

So far, it has been assessed the accuracy and completeness of current nuclear data that are used to calculate material radiation damaging. **The fourth objective** of this work is to assess:

- the potential impact of the **uncertainty in the efficiency factor** provided by the OECD/NEA primary damage group
- the potential impact on **nuclear data uncertainties** in the damage energy cross-section

Regarding **the first uncertainty issue**, the variables "b" and "c" in the formulation of $\zeta = f(b,c)$ will be assumed as random variables with the probability density function provided by the OECD/NEA primary damage group. Then, a sampling of n-NJOY cases will be run to calculate average, deviation and correlation matrix for the damage energy cross-section.

Regarding **the second uncertainty issue**, the technique applied will be the Monte Carlo approach using a large number of random ENDF files taken form TENDL library. The TALYS code and the randomly generated cross section evaluations available within the TENDL-2012 cross section library make it possible to explore this approach. The TENDL-2012 random library with enough sample size (>500 files for the random cross-section) is used in order to generate a good statistical analysis in a multigroup energy structure. Additionally to damage energy cross-sections, gas (He and H) production cross sections will be processed as a component of primary damage. At present, TENDL-2012 shows a relative error of ~25% and ~18%, for Fe(n,xα) and Fe(n,xH), respectively.

Other uncertainty methodologies will be explored in order to generate a consistent data of damage energy-cross section and their uncertainty. However, any work performed with TENDL-20xx to evaluate uncertainties cannot be directly extrapolated to any other library.

This uncertainty analysis will be complemented with a sensitivity analysis to predict the most important reaction channel contributors to the damage energy-cross section.

Finally, to assess the impact of these uncertainties in a particular application, the spectrum averaged displacement cross-sections $\langle \sigma_d \rangle = \int \sigma_d(E)\phi(E)dE / \int \phi(E)dE$) will be used for different neutron environments. For instance, it has been reported that for a neutron spectrum of the MFE/DEMO First Structural Wall with a hard neutron spectrum (averaged energy ~3.8 MeV), there can be predicted a low value of uncertainty ~ 2% when TENDL2012 libraries are used.

Using NJOY to Calculate "Damage" with Modern Evaluated Nuclear Data Files

A. C. (Skip) Kahler

T-2, Nuclear and Particle Physics, Astrophysics and Cosmology Group
Theoretical Division
Los Alamos National Laboratory
USA

Evaluated nuclear data files such as ENDF/B (United States), JEFF (Europe), JENDL (Japan), CENDL (China), etc. are a source of fundamental particle + target nuclear interaction data. These data can include (i) resolved and unresolved resonance parameters, (ii) pointwise reaction cross sections for

a variety of specific reactions, (iii) angular distributions of the outgoing particles, (iv) energy spectra of the outgoing particles, (v) prompt, delayed and total fission nu, (vi) photon emission data and more. Evaluated files with sufficient information to perform detailed radiation transport calculations are referred to as "General Purpose" files. Other compilations focus on a more limited set of nuclear data, suitable perhaps for determining reaction rates under known irradiation conditions. These are referred to as "Special Purpose" files. Examples include the European Activation File, EAF-2010 and the IAEA's International Reactor Dosimetry and Fusion File, IRDFF, which is currently the subject of its own CRP.

What is not provided in evaluated data files are KERMA (Kinetic Energy Release in MAterials), total gas production cross sections, and "Damage" cross sections. These quantities are sometimes characterized as "derived" quantities since they are obtained via a processing code, such as NJOY [1], that utilizes the fundamental data found in a General Purpose file.

During the 1st RCM meeting presentation a review of the basic ENDF-6 format was given. That review is not repeated here, rather we assume the reader already understands the basic terminology such as "mf" and "mt" number associated with an ENDF formatted evaluation. NJOY's capability for calculating KERMA was reviewed at the Technical Meeting preceding formation of this CRP, and was not repeated during this meeting.

As implied above, a General Purpose evaluation may consist of many different reactions, each identified by a unique "mt" number. In order for an End-User of these data to determine a quantity of interest such as gas production it is necessary to add all the mt numbers that include the requisite outgoing particle (i.e., p,d,t,^{3}He or α), including a multiplicity factor when two or more of the outgoing particle is produced, while omitting redundant mt values (such as don't include any of mt800 through mt849 if mt107 is present). NJOY's GASPR module can be used to perform these summations, and will output using mt=203 through 207 a cross section representing the p, d, t, ^{3}He and α particle production cross section, respectively, from all other mt reactions that were defined within a given evaluation. The 203 through 207 mt values are defined in the ENDF format for this purpose and so any further processing desired by the End-User of these data by any ENDF processing code should occur without incident.

Radiation damage in a material is often characterized by "DPA", or Displacements per Atom. Norgett, Robinson and Torres (NRT) proposed a model to calculate DPA in the mid-1970s, where

$$DPA = \frac{0.8E_a}{2E_d}.$$

E_d is the energy needed to displace an atom from its lattice position. Typical values, by element, range from 25 eV to 90 eV. Values for 22 elements are hardwired into NJOY, with a default value of 25 eV used for the remaining elements. These values can be overridden by User input. E_a represents the energy available to disrupt the lattice due to the energy of the incident particle and the specifics of the nuclear interaction. E_a is further modified since some energy loss occurs due to electronic excitation. The Robinson partition function, P(E), due to the electron screening theory of Lindhard is used by NJOY. The specific formula [2,3] is

$P(E_R) = \frac{E_R}{1+F_L\left(3.4008\varepsilon^{1/6}+0.40244\varepsilon^{3/4}+\varepsilon\right)}$, or zero if $E_R \leq E_d$

where

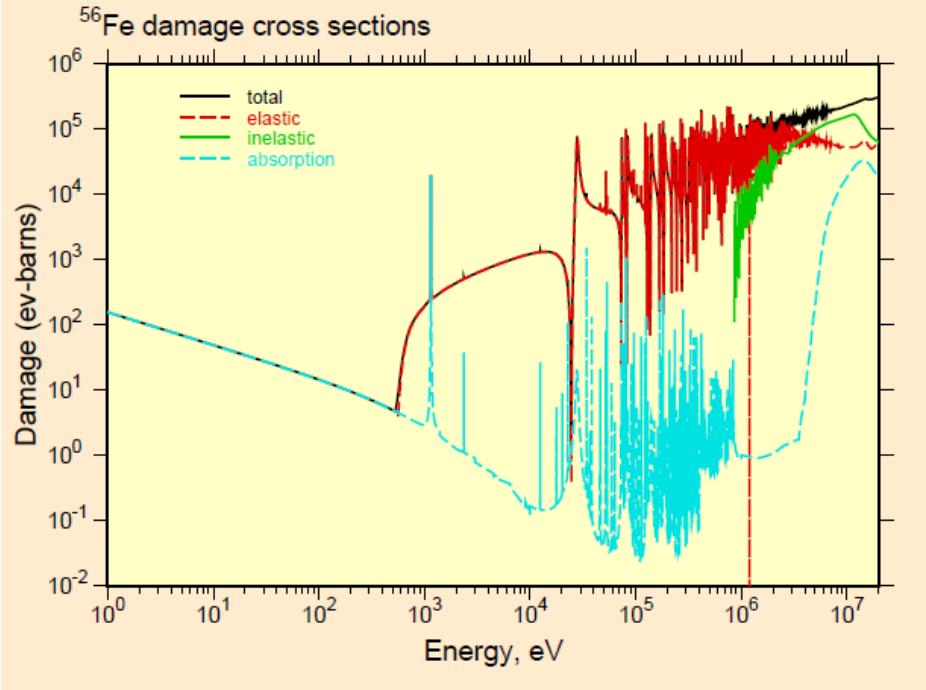
$\varepsilon = \frac{E_R}{E_L}$,

$E_L = 30.724 Z_R Z_L \sqrt{Z_R^{2/3} + Z_L^{2/3}}\,\frac{(A_R+A_L)}{A_L}$,

$F_L = \frac{0.0793 Z_R^{2/3} Z_L^{1/2} (A_R+A_L)^{2/3}}{\left(Z_R^{2/3}+Z_L^{2/3}\right)^{3/4} A_R^{3/2} A_L^{1/2}}$, and

Z_i and A_i are the charge and atomic number of the lattice (L) and recoil (R) nuclei, respectively.

The requisite nuclear data, including reaction Q value, outgoing particle angular distributions and energy spectra and associated photon emission are extracted from the evaluated nuclear data file. The specific formulas used for (i) elastic and discrete level inelastic scattering, (ii) continuum reactions, (iii) capture (i.e., (n,g)) and (iv) particle emission were discussed during the meeting, have been published elsewhere [1,4] and so are not repeated in this brief summary. It is clear that the total damage cross section calculated by NJOY will contain a number of components, one for each mt number. NJOY collapses these components into various categories, including "total", "elastic", "inelastic" and "absorption". Examples of NJOY's calculated damage cross sections were shown during the meeting, for ENDF/B-VII.1 ^{27}Al and ^{56}Fe. The ^{56}Fe plot is reproduced here.



The methodology employed by NJOY for "damage" calculations was developed in the early 1980s [5,6] and is virtually unchanged since that time. We stand ready to implement revised algorithms in the production version of NJOY2012 that reflect consensus, state of the art, methods as recommended by this CRP. Furthermore, test versions of NJOY2012 can be developed to compare the results of revised models and theories that may be proposed during this CRP.

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Post-Meeting Note. The IAEA Nuclear Data Section noted during this meeting that a special data library, DXS, containing gas production and displacement cross sections was available for a selection of materials. The data provided within these files conforms to the ENDF-6 mf=3 format, and the gas production data use the ENDF defined mt = 203 through mt = 207 values. However, the model dependent displacement cross sections utilize currently undefined mt numbers; mt = 900 for

displacement cross sections derived from a combined binary collision approximation/molecular dynamics simulation, and mt = 901 for displacement cross sections based upon the NRT model. The standard version of NJOY2012's GROUPR module will not process undefined mt sections in an ENDF formatted file, but a simple code patch will overcome this limitation. We do not expect to implement this code patch in the production version of the code, but upon request can make it available to licensed NJOY2012 users who are supporting this CRP.

Recommendations and Research Summary for IAEA Coordinated Research Project on Primary Radiation Damage Cross Sections

Roger E. Stoller

Materials Science and Technology Division
Oak Ridge National Laboratory
USA

Objective:

The objective of this presentation was to describe the author's recommendations for work scope in the IAEA Coordinated Research Project (CRP) on Primary Radiation Damage Cross Sections and describe the research activities in which he will engage to further objectives of the CRP.

Previous Research and Recommendations:

The two most common parameters used to characterize the cumulative exposure of a material to irradiation are the particle fluence and absorbed dose. The **particle fluence**, in units of $(\text{area})^{-1}$, depends only on the characteristics of irradiation source and can be quoted at a point or averaged over a surface or volume. The **absorbed dose,** in units of energy, depends on a variety of variables, including: particle fluence, particle type, particle energy spectrum, and the specific material being exposed. Thus, absorbed dose includes much more information about the irradiation environment, and it is material dependent.

Both particle fluence and absorbed dose are used as independent variables in attempts to correlate data, compare materials or irradiation environments, or extrapolate data to estimate the effects of a longer exposure. This use as a **damage correlation parameter** introduces a much broader range of influences than simply the material and the irradiation source. In general, the application of a damage correlation parameter will depend on: the particle fluence or absorbed dose, specific damage parameter being monitored (e.g. electrical resistivity, swelling, or embrittlement), the damage rate, previous damage, exposure conditions such as temperature and mechanical loads, and material composition (intentional alloy elements and impurities). The impact of correlated damage mechanisms such as transmutation production, notably helium and hydrogen, must also be considered.

In spite of its limitations, the secondary displacement model of Norgett, Robinson, and Torrens (NRT) has been a de facto standard in the nuclear materials research community since its introduction in 1975 [1]. The NRT model provides a procedure for estimating of the number of atomic displacements per atom (dpa) due to the kinetic energy the atoms in a material absorb during exposure to high energy particles, the so-called damage energy. Based on modern molecular dynamics (MD) simulations and cryogenic irradiation experiments, it is clear that the number of stable vacancies and interstitials formed in irradiated materials is about 20 to 40% of the NRT value [2]. Previous work, shown in Fig. 1, has developed modifications to the NRT dpa that appear to provide a better estimate of stable Frenkel pair production in iron, as well as other damage parameters related to in-cascade clustering [3,4].

However, it must be remembered that the MD simulations are effectively carried out using computationally pure metals which do not exist in nature. Results were presented that illustrated how the presence of defects, grain boundaries, and free surfaces can influence defect formation in displacement cascades. In addition, the experimental data that are of interest for correlation involves irradiation experiments which last from days to years, while a displacement cascade lasts about 10^{-11}

sec. Thus, a broad range of phenomena such as long-range defect diffusion and defect aggregation occur after the cascade and ultimately determine the radiation-induced property changes. As a result, it is unlikely that a single, simple radiation exposure parameter can function as a damage correlation parameter for the many radiation-induced phenomena of interest. Moreover, there a range of materials and material properties for which atomic displacements are not the primary source of damage, notably the physical properties of covalent and ionic materials for which the ionizing dose is more important than the displacement dose. Nuclear transmutation products, both gases and solids, are also critical in some cases.

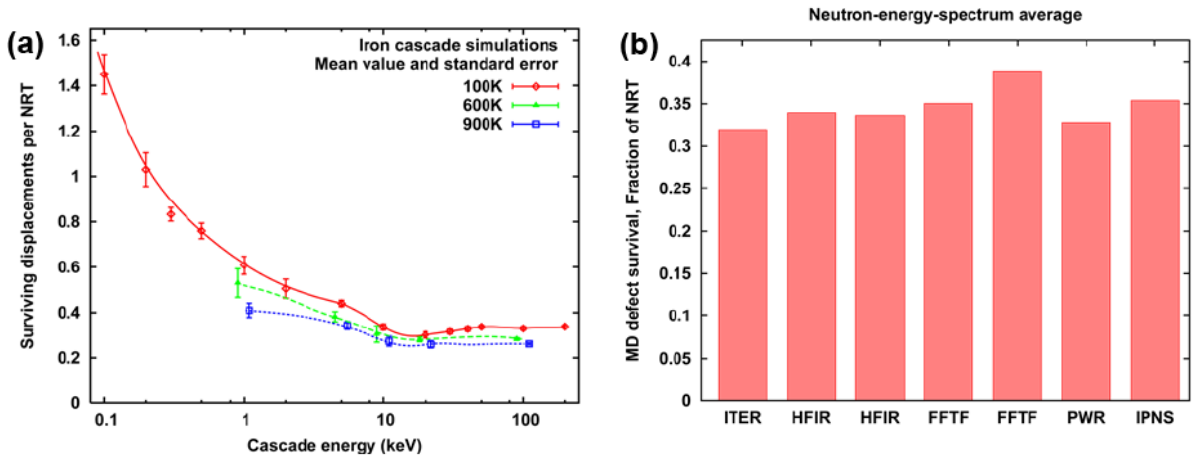

Fig. 1. Energy and temperature dependence of defect formation in MD simulations (a) and spectrum-averaged production values for the indicated irradiation environments (b) relative to the NRT displacements [2, 3, 4].

The damage energy, which is the kinetic energy deposited in elastic collisions with lattice atoms is employed in the NRT model as shown in Eqs. (1) to estimate of the number of displacements (Frenkel pair) created by a given primary knock-on atom:

$$\nu_{NRT} = \frac{0.8T_d}{2E_d} \qquad (1)$$

where *Td* is the damage energy, *Ed* is the minimum energy required on average to create a stable Frenkel pair, the factor of 0.8 was determined from binary collision models to account for realistic (i.e. not hard sphere) scattering. The damage energy in Eqn. (1) is obtained using the energy partitioning theory developed by Lindhard, et al. [5]. Since the damage energy is the only parameter in Eqn. (1) that can be determined from nuclear reaction theory, it is recommended that one component of the CRP should focus on obtaining the best possible values for this fundamental quantity. A second component should involve the development of materials damage response functions that may prove to provide better correlation parameters than the simple NRT dpa. For example, some mechanical property changes may be better correlated using a quantity related to the point defect clusters that are formed in displacement cascades.

ORNL Contribution to the CRP

Within the CRP, the presenter will collaborate with other participants to carry out MD cascade simulations and the necessary analysis to develop the additional damage response functions. The general approach with be that followed in Refs. 3 and 4, but will extend to the range of materials identified as of interest to the CRP. Both existing databases of MD cascade simulations and new simulations will be employed.

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Quantifying primary irradiation damage from cascades to characterize the long-term behaviour of its accumulation

Chung H. Woo

Department of Physics and Materials Science
City University of Hong Kong
Hong Kong SAR
China

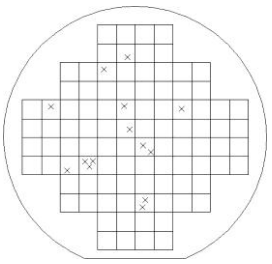
1. Introduction

High-energy recoil events in a crystalline solid due to fast fission or fusion neutrons result in the (near) simultaneous creation of a large number of atomic displacements in a small cascade volume. This mode of displacement damage production gives rise to two important effects. Firstly, extensive annealing occurs, which only allows a fraction of the initial displacements to survive as vacancies and interstitials, as well as their clusters. Early investigations of cascade morphology concentrated on the intra-cascade clustering of vacancies. Using a diffusion-reaction formulation to account for clustering, Woo, Singh and Heinisch (1990) looked into the recombination and clustering of interstitials in a cascade and discovered that a significant fraction of the interstitials produced in a cascade could be immobilized in the form of clusters. This picture of cascade damage led Woo and Singh (1990, 1992) to the formulation of the Production Bias model, from which it became obvious that irradiation damage accumulation depended quantitatively on in-cascade survival probabilities and clustering fractions. Trinkaus *et al*. [1994] reviewed the experimental evidence and concluded that all available observations were consistent with the premise of interstitial cluster formation. Subsequent molecular dynamics studies of cascades by many authors also confirmed the formation of intra-cascade interstitial and vacancy clusters. More importantly, that the fraction of vacancies in the PVCs was not exactly the same as that of interstitials in the PICs was also confirmed. To obtain a quantitative description of these factors in various metals and alloys naturally becomes a favoured objective of studies of primary irradiation damage pursued by many authors.

The second effect is more subtle and has received much less attention. It originates from the strong temporal and spatial correlations of point-defects produced in the same cascade. Indeed, as a result of random cascade occurrence, production of point-defect is not deterministic and continuous, but probabilistic and in discrete packages (Semenov and Woo 1993, 2001). It is intuitively clear that fluctuations in point-defect concentrations are of primary importance in processes that involve only a small number of point-defects. Examples are the long-term evolution of the in-cascade clusters, the nucleation of various microstructure elements, such as voids and interstitial loops. Indeed, an interstitial cluster that has been annihilated due to a surge of vacancies cannot be revived by interstitials that arrive afterwards, even though the wave of interstitials may be bigger. The clarification of the role played by the strongly correlated production mode of point-defects in cascades, the identification of the related parameters, and the construction of a physically transparent and easy to use model to account for this effect, are very much needed to complete the research on

Primary Radiation Damage from nuclear reaction to point-defects. This is the objective of the present investigation.

2. Dpa-rate fluctuations



The number of point defects generated by cascades in a volume ΔV and time Δt is not a constant, but a fluctuating quantity as a result of the probabilistic nature of random cascade occurrence (see figure). Cascade initiations by separate incident particles are independent events, so that cascade events in the same volume at different times or between cascade events in different volumes at any time are not correlated. The probability of occurrence of μ cascades in $\Delta t \Delta V$ can be described as a Poisson distribution under the condition that $<\mu> < 1$, which is satisfied when $\Delta t \Delta V$ is sufficiently small.

Suppose N_G is the number of PKA energy groups, and N_p the average number of point defects produced by a PKA of group p ($p = 1,\ldots, N_G$). If μ_p is the number of cascade occurrence in $\Delta V \Delta t$ due to PKAs of group p. Then the total number of point-defects m generated in $\Delta V \Delta t$ is given by

$$m = \sum_{p=1}^{N_G} \mu_p N_p \equiv \frac{G \Delta V \Delta t}{\Omega} \tag{1}$$

The statistics of point-defect production can be worked out from the statistics of m. Thus,

$$\frac{\bar{G} \Delta V \Delta t}{\Omega} = \langle m \rangle = \langle N_p \rangle \left\langle \sum_{p=1}^{N_G} \mu_p \right\rangle = \langle \mu \rangle \langle N_p \rangle \tag{2}$$

where the mean $\langle N_p \rangle$ is obtained from the average of the point-defect production efficiencies weighted by the PKA spectrum. Using Eq. (1), the variance of m is given by,

$$\begin{aligned} &Var[m] = Var[\mu N_p] \\ &= \langle \mu \rangle^2 Var[N_p] + \langle N_p \rangle^2 Var[\mu] + Var[\mu] Var[N_d] \\ &= \langle \mu \rangle^2 Var[N_p] + \langle \mu \rangle \langle N_p^2 \rangle \end{aligned} \tag{3}$$

From Eqs. (2), in the limit $\Delta V \Delta t \to 0$, eq. (3) can be written as

$$\langle (\delta m)^2 \rangle = \frac{\bar{G} \Delta V \Delta t}{\Omega} \frac{\langle N_p^2 \rangle}{\langle N_p \rangle}$$

Using this result, the variance of G can be expressed in terms of the cascade characteristics:

$$\langle (\delta m)^2 \rangle = \left\langle (\delta G)^2 \left(\frac{\Delta V \Delta t}{\Omega} \right)^2 \right\rangle = \bar{G} \frac{\Delta V \Delta t}{\Omega} \frac{\langle N_p^2 \rangle}{\langle N_p \rangle}$$

$$\Rightarrow \langle (\delta G)^2 \rangle \Delta V \Delta t = \bar{G} \Omega \frac{\langle N_p^2 \rangle}{\langle N_p \rangle}$$

From the foregoing, the point-defect generation rate $G_j(\mathbf{r},t)$ is a stochastic variable with mean value $\langle G_j(\mathbf{r},t) \rangle = \bar{G}_j$ and fluctuations $\delta G_j(\mathbf{r},t)$, which obey $\langle \delta G_j(\mathbf{r},t) \rangle = 0$ and have correlation function given by

$$\langle \delta G_j(\mathbf{r},t) \delta G_j(\mathbf{r}',t') \rangle = \bar{G} \Omega \frac{\langle N_p^2 \rangle}{\langle N_p \rangle} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \cdot$$

In rate-theory type of irradiation damage modeling, $\bar{G}_j$ determines the rate of microstructure evolution and macroscopic effects such as swelling rate, creep rate, growth rate, etc., while the difference between the $\bar{G}_i$ and $\bar{G}_v$ provides the production bias. The fluctuations provide the non-equilibrium activation entropy to overcome the nucleation barriers in the classical nucleation theory. They have to

be taken into account in the study of irradiation damage accumulation beyond the mean-field model, such as the Fokker-Planck equation approach or the mater equation approach or field theory approach.

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Development of Fe-Cu-Ni-Mn potential for study of the primary damage in model alloys for Reactor Pressure Vessel steels

D. Terentyev

Centre d' Etude de l'Energie Nucleaire
Boeretang 200
2400 Mol
Belgium

Relevance of the present contribution

The displacement cross section is a reference measure used to characterize and compare the radiation damage (in terms of lattice defects) induced by neutrons and charged particles in crystalline materials. Norgett-Torrens-Robinson (NRT) standard [1] proposed almost 40 years ago has been recently revisited with the aid of modern computer simulation techniques such as combination of Molecular Dynamics and Monte Carlo simulations (for review in Iron see [2]), based on the interatomic models fitted using first principle calculations and experimental data. In the case of such important nuclear material as body centered cubic Iron (BCC Fe), it has been shown that the number of survived defects as compared to the NRT prediction is systematically lower and the discrepancy depends on the recoil energy [3]. A similar result was obtained for BCC Fe-Cr solid solution [4]. These studies have clearly demonstrated how modern computational material science techniques may contribute to the upgrade of nuclear cross-section database as well as in general to the understanding of primary radiation damage process and state in metallic materials.

Most of the studies performed in bcc Fe were in fact addressing Fe-based structural alloys among which there are high-Cr steels (for fusion and GEN IV reactors) and Reactor Pressure Vessel (RPV) steels. The primary radiation damage phenomenon (PRD) in the latter type of steels is the subject of the present contribution. The need to understand radiation damage in RPV steels is driven by the radiation-induced hardening which must be kept at the acceptable level for the safe exploitation of the vessel (see e.g.[5]). Historically, the hardening was associated to the formation of Cu-containing precipitates (accelerated by the radiation produced defects), hence Fe-Cu binary was taken as model material for RPV steels [5]. With the appearance of fine microstructural characterization techniques it has been recognized that Cu-precipitates formed under irradiation contain significant amount of vacancies [6; 7], so pure Cu precipitates formed upon thermal ageing are not representative to study embrittlement of RPV steels. At the same time, an in-depth mechanical and microstructural characterization concluded that experimentally measured hardening in RPV steels can not be explained by the detectable microstructural features and further detailed investigation of the invisible damage needs to be assessed [8]. Application of Topographic Atom Probe and Positron Annihilation Spectroscopy provided new information on chemical composition of agglomerates, possibly responsible for the hardening. Analysis of different types of RPV steels revealed the presence of Mn and Ni enrichment [9]. That information has totally fitted in the conventional correlation models applied to assess the hardening in RPV surveillance programme [10]. However, what is the atomic structure of the defects containing high percentage of Mn and Ni remained unclear.

A massive campaign combining experimental and theoretical studies has been initiated in the frame of FP7 European programme (EP 'Perform60'), addressing the issues of safety of Light Water Reactors and prolongation of their lifetime. A number of experiments, addressing evolution of microstructure and subsequent hardening in Fe, Fe-Cu, Fe-Mn-Ni, PRV steel, were performed [9]. The experiments did not reveal the presence of visible damage in RPV steels, while dislocation loops were observed in all model alloys. The numerous formation Mn-Ni-rich clusters was confirmed in model alloys and RPV steel. Importantly, the density and size of invisible defects is comparable in the model alloys and RPV steel. Eventually, hardening in pure Fe and model alloys is severely determined by the formation of TEM-visible dislocation loops, while their growth is somehow suppressed in RPV steel (which also shows essential hardening). One may therefore assume that solute-rich clusters containing Mn and Ni atoms are associated with small but numerous dislocation loops (with mean distance reaching 10 nm), which at the end significantly contribute to the hardening of RPV steels.

If one accepts this picture, every high energy cascade event will occur in the material containing a high density of pre-existing nano-voids and dislocation loops. What could be the role of the pre-existing nanostructural defects (significantly enriched with solutes) in the establishment of the primary damage state is the subject of this contribution. To address this question it is necessary to understand most probable structures of these solute-rich clusters and their arrangement on small dislocation loops, which would be subject for displacement cascade simulations. Naturally, these atomic scale studies will require a reliable interatomic potential. Below, the recently developed Fe-Cu-Ni-Mn many body interatomic potential for RPV model alloys is described.

Development of Fe-Cu-Ni-Mn interatomic potential

All details regarding the development of the interatomic potential are described in our recent work [11]. Here we concentrate only on the essential features that were considered in the process of the derivation. The potential is made using Embedded Atom Method formalism [12] and itself it is a central force many body potential. The Fe-Cu and Fe-Ni-Cu potentials were developed in the preceding years and the main accent was made on the correct solubility limit of Cu and Cu-Ni, and in general on the consistence with the thermodynamic behaviour [13]. A number of Monte Carlo studies has shown that the precipitation of Cu in Fe-Cu and in Fe-Cu-Ni alloys is very well described by the potentials, concluded on the basis of the agreement with experiments [14; 15]. The Fe-Cu-Ni potential was also exploited for the investigations of the hardening due to Cu-vacancy-rich clusters (with and without Ni) [16]. There it was concluded that hardening due to Cu-rich vacancies is not sufficient to explain the experimental result in RPV steels. The interaction of point defects and solutes was carefully fitted using *ab initio* data (and some limited experimental evidence). The quaternary FeCuNiMn potential is based on the extensive DFT dataset on solute–solute and solute-point defect interaction. Certain experimental data (e.g. phase diagrams) were used to validate the potential. The reference DFT data on solute–solute interaction reveal that, while Mn–Ni pairs and triplets are unstable in bcc Fe matrix, larger clusters are actually kept together by the collective attractive interaction. That implies that initial seeds for the nucleation of Mn-Ni clusters are necessary to induce a considerable segregation (as obtained experimentally). Thus, the formation of thermodynamically stable Mn–Ni-rich phases in Fe is actually possible under cascade damage irradiation, which generate nanometric dislocation loops, proven to be strong enough defects to induced heterogeneous nucleation of solute clusters [11].

Outlook

In this project, we will extend the research on primary damage effects by considering Fe-Cu, Fe-Ni, Fe-Mn and Fe-Cu-Ni-Mn alloys. The composition of the alloying elements will be chosen so as to be relevant for RPV steels. As a next step, we assess how the presence of solute-rich clusters, associated either with interstitial type defects or with vacancy clusters, affects the primary damage state. And vice versa, stability of the solute-rich clusters under collision cascades will be studied. A parametric MD study will be done to investigate the evolution of collision cascades in the crystals containing Cu-vacancy-rich clusters (as experiments directly suggest) and Ni-Mn solutes associated to dislocation loops (as recent atomistic studies suggest). The effect of these nano-structures on the total number of survived Frenkel pairs, their clustered fraction, morphology of point defect clusters etc. will be studied

using the above described potential. The impact of cascades will be investigated at room temperature and 300°C varying the recoil energy from 10 up to 200 keV.

As a result, we expect to provide data which will contribute to further understanding of the primary damage formation and annealing in BCC Fe-based alloys relevant for nuclear applications. The uncertainly attributed to the survived PRD and clusterization of point defects will be evaluated. Finally, the existing knowledge on primary damage state will be extended to Fe-Cu and Fe-Cu-Ni-Mn alloys.

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Beyond NRT concept: using BCA codes to design irradiation experiments to emulate neutron fusion effects in materials

F. Mota, C.J. Ortiz, R. Vila

Laboratorio Nacional de Fusión – CIEMAT, Material group
Madrid
Spain

1. Brief description of the work development so far

A methodology was developed to calculate the damage due to fusion neutrons in Materials (monocrystal, polycrystal and amorphous systems). This methodology is based on one developed by KIT laboratory [1, 2]. It consists of a combination of Nuclear Data Libraries Processing, Neutronics transport and Monte Carlo Binary Collision codes.

This methodology allows designing irradiation experiments with ions or neutron to emulate neutron fusion effects in materials in better way than NRT method [3]. It is possible because the displacement damage generation have been calculated using the same methodology for both neutron and ion irradiations (starting from PKA spectra). The block diagram is shown in Fig. 1.

The resulting damage profile used to calculate damage function and damage dose was calculated using MARLOWE code [4, 5].

MARLOWE code shows to be of high interest to simulate displacement cascades in monocrystal, polycrystal or amorphous materials. It allows exploring higher energies (up to GeV) in a much shorter time than MD. It represents thus an interesting alternative to MD to simulate the effects of energetic fusion neutrons in materials. In order to accurately predict the number of stable Frenkel pairs produced in cascades, those that will contribute to the long-term evolution of defects, the I-V capture radius must be first calculated. This can be done using MD results obtained for low-medium PKA energies (~ keV). As an example, the capture radius of I-V pairs in Fe as a function of PKA energy has been calculated [6]. MARLOWE is able to account for the recombination of defects that occur during the cooling phase of a cascade by means of the concept of capture radius. A constant capture radius of about 3.3 Â was obtained for energies higher than 5 keV. MARLOWE can thus be used to simulate displacement cascades with energies higher than 5 keV in Fe with this calibrated value of the capture radius. For lower PKA energies it was observed that the capture radius is variable and must be determined for each PKA energy.

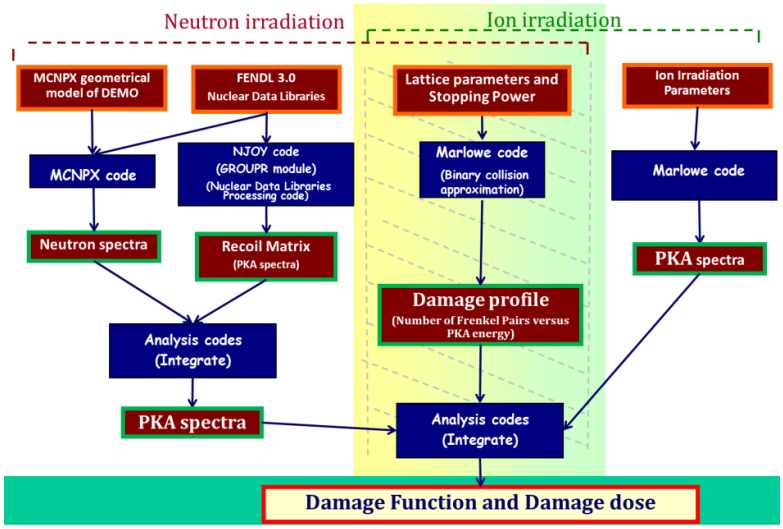

Figure 1. Methodology block diagram.

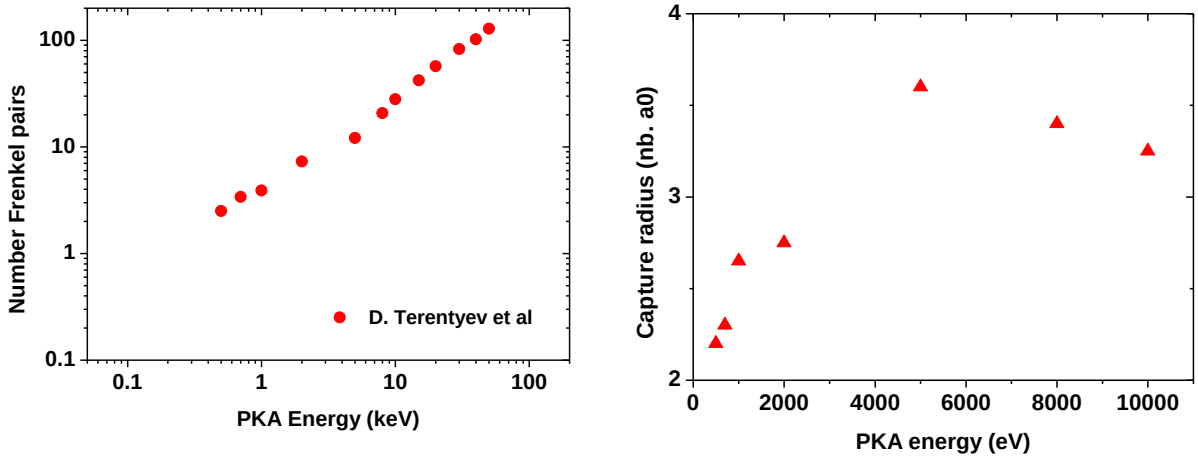

Fig. 5. **Left**: Molecular dynamics simulations provided by D. Terentyev used to fit the capture radius for MARLOWE code; **Right**: Radius capture as a function of PKA energy determined for MARLOWE comparing with MD simulations.

2. WORK Plan for the next three years

An extension to insulators is needed, as the NRT method has been validated mainly for metals. Therefore, we need molecular dynamics simulations for insulators to fit the capture radius, for example for:

- Al_2O_3: As a major candidate as general insulator and tritium permeation barrier in DEMO;
- SiC: Used as "Flow Channel Inserts (FCI's)" for DCLL DEMO concept;
- SiO_2: used for diagnostic windows, fibre optics, etc.

As first step, collaboration with Dr. Kai Nordlund was proposed. It is based on using their MD results as an input to MARLOWE to calculate the capture radius for SiO_2 and its evolution with irradiation parameters.

In addition, we are planning to develop MD calculation for Al_2O_3. Currently these simulations are in progress updating the code to deal with this problem; therefore, it is our intention for the next year to have preliminary results.

We shall also explore the possibility to work on SiC, since it is a functional material of great interest in the nuclear fusion development program. But it is a lower priority task. However, this part of the work is subject to the obtaining of MD results on SiC.

Therefore for the next three year we propose:

Work Plan for the first year

For the first year of the project, we propose to use MARLOWE code to determine the I-V capture radius in Fe, SiO_2 and Al_2O_3 as a function of PKA energy. To do so, BCA simulations will be run and compared to MD simulations for a range of PKA energies. For each energy, the corresponding capture radius will be extracted by fitting the BCA result to the one obtained by MD. MD simulations will be performed in a parallel task of the present project. In addition to the value of the capture radius that will be obtained and that will be useful for future BCA simulations, this will allow to determine whether the capture radius varies with the PKA energy or not. The case of Fe has already been achieved and results were presented in this first CRP meeting.

Work Plan for second year

During the second year of project we shall determine the PKA spectrum generated in Fe, SiO_2 and Al_2O_3 by irradiation at different energies and different neutron and Ion facilities. It will be obtained for different nuclear data libraries to assess the nuclear data included in each data libraries.

Work Plan for third year

During the third year of the project, MARLOWE code will be used to determine damage profile, i.e. the number of Frenkel Pairs versus PKA energy, for the materials evaluated. This damage profile is the key parameter to be able to determine the primary displacement damage dose (dpa values) and damage function induced by different irradiation facilities (neutron source and ion irradiation) and calculated using the methodology described above.

In addition, attempts will be made to validate the results obtained with MARLOWE code with available data in the literature.

3. Proposals to standardize the method

For the duration of the program (three or four year), we are going to look for the best way to standardize the proposed methodology, Figure 1, to be used easily for different users, as one of the main deliverables of this project.

Reference

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The improvement of solid target reaction cross-section investigation method and first preliminary results

I.P. Bondarenko, V.A. Khryachkov, T.A. Khromyleva, B.D. Kuzminov, N.N. Semenova and A.I. Sergachev

Institute for Physics and Power Engineering
Bondarenko Ploshad 1, Obninsk
Russian Federation

The double back-to back ionization chamber with Frisch grid is the detector in our method. The working gas is 97% Kr + 3% CH_4 gas mixture under absolute pressure of 3 bar. The ^{238}U layer in the non-grid chamber was used for monitoring neutron flux. The uranium target has 99.99% enrichment of ^{238}U isotope and has mass of 4.60 mg. The dead time in main and monitor channels was identical due to features of used method. So neutron flux was measured in the area close to investigating target. The spacing between ^{238}U and target layers was taken into account on data processing stage.

The chromium solid target with surface density 365 μg/cm^2 was used for the $^{50}Cr(n,\alpha)^{47}Ti$ reaction cross section investigation. The isotopic composition of the target is ^{50}Cr – 96.8%, ^{52}Cr – 2.98%, ^{53}Cr – 0.18%, and ^{54}Cr – 0.04%. Full target mass is 5.15 mg and it is placed on 84 mg/cm^2 thickness gold foil.

The chromium solid target with surface density 280 μg/cm^2 was used for $^{52}Cr(n,\alpha)^{49}Ti$ reaction cross section investigation. The target spot diameter is 30.9 mm, gold backing is 190 mg/cm^2 surface density. The isotopic composition of the target is ^{50}Cr – 0.1%, ^{52}Cr – 99.5%, ^{53}Cr – 0.3% and ^{54}Cr – 0.1%. Full target mass is 2.1 mg.

The experiments with cathode target placement, made obvious huge background from cathode material and α-particles from reactions on oxygen and nitrogen compositions on cathode surface, so the investigating effect is almost lost in the background. To avoid such effect the target was placed on gold threads, fixed with the first guard electrode – 1 cm spatial separation of target from cathode was achieved. Gold threads were not only for physical support, but for electrical potential to be regular. Summarizing all mentioned above – it became possible to select target α-particles from the gas α-particles (Fig. 1).

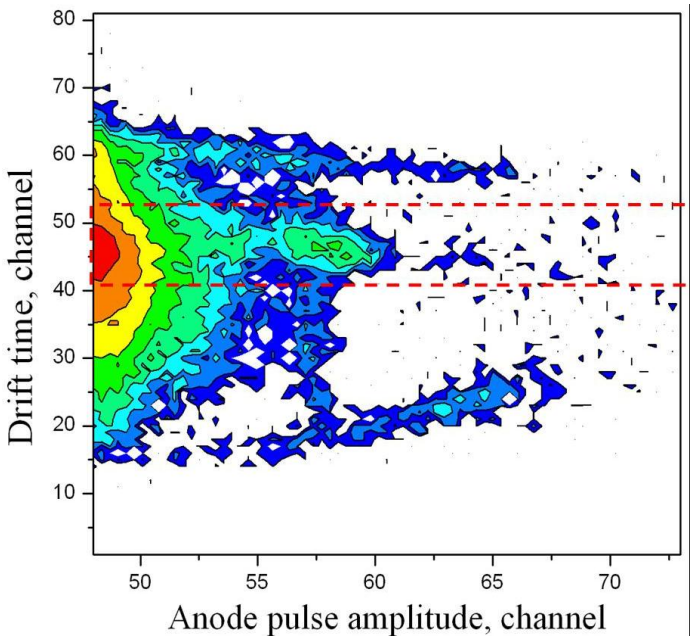


Figure 1. Three dimensional spectrum with clear area of target events.

Electron drift time depends on the distance they need to pass before been collected on the anode. And that is how we can separate particles by their birth place to reduce the background from parasitic

reactions. It should be mentioned that all named procedures can be made by digital signal processing methods.

Analog signals from the anode and the cathode of the ionization chamber go to preamplifiers, then wave form digitizer (LeCroy 2262) where turned to digital data for further processing. This processing is made by our self written programs, so we can get different data from digitized signals (Fig. 2).

Digital Signal Processing allows us to analyse: anode pulse amplitude (PA); cathode pulse amplitude (PC); moment of time when cathode signal appear (TSC); moment of time when anode signal appear (TSA); moment of time when anode signal reach satiation (TEA); time of charges movement in ionizing chamber Td = (TEA- TSC); anode signal rise time Tr = (TEA- TSA) Birth place X = (D-Td*Ve). Complex analysis of all mentioned parameters gives us information about energy of registered particle, its birthplace and type. These parameters allow us to decrease the background and increase the reliability of determination of events from the reaction under investigation.

Counting statistics consists of number of the α-particles uncertainties and number of the fission fragments. Errors not related to statistics:

– α-particles "tail" extrapolation – 0,4%.

– Fission fragments "tail" extrapolation – 0,6%.

– Number of ^{238}U atoms – 1,5%.

– ^{238}U cross section – 1%.

– Number of chromium atoms – 3,2%.

– Total errors not related to statistics – 3,7%.

– Typical statistical uncertainty from 2 to 15 %.

All the experiments will be carried out on electrostatic accelerator EG-1 of Institute for Physics and Power Engineering, Russia. Neutrons are generated from D(d,n) reaction on titanium-deuterium target with thickness 1 mg/cm^2.

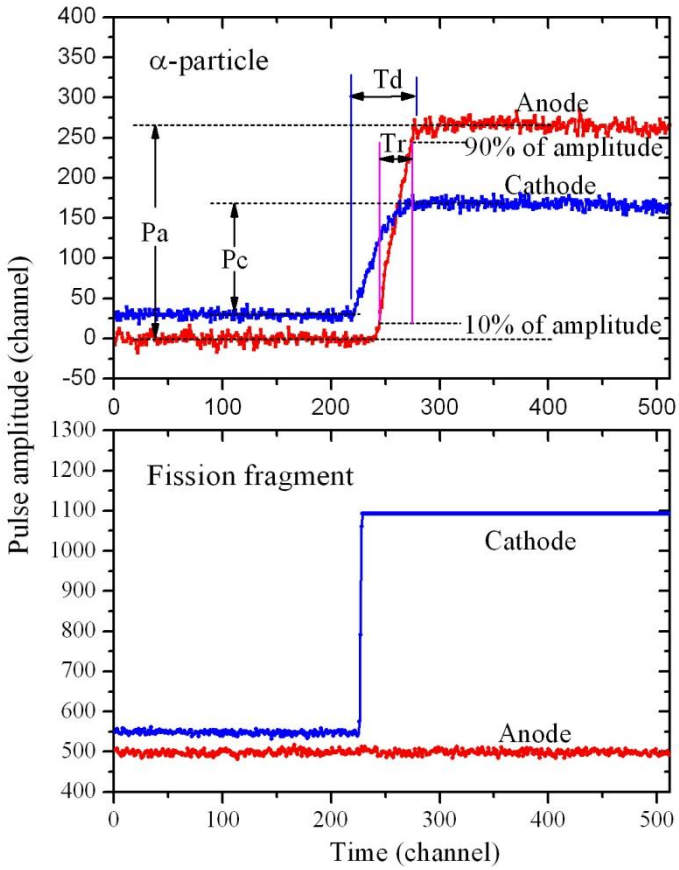


Figure 2. Signals examples with parameters we use in data processing

The preliminary results of $^{50}Cr(n,\alpha)^{47}Ti$ reaction cross section are represented on Figure 3.

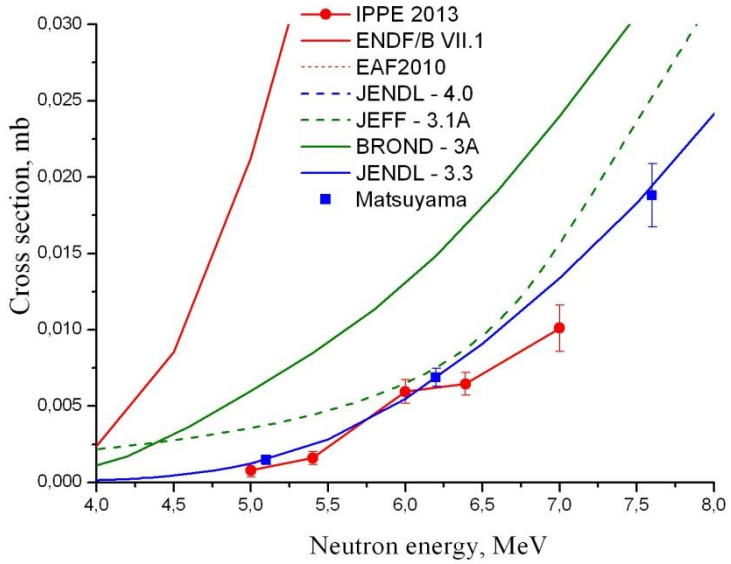


Figure 3 Preliminary results of $^{50}Cr(n,\alpha)^{47}Ti$ reaction cross section.

First year work plan:

- detector upgrade for decreasing of its construction elements input in background by replacing stainless steel elements with cadmium ones;
- making the cathode–target spatial separation by placing target on gold threads;
- measurement of (n, α) reaction cross section in 5–7 MeV neutron energy range.

Primary damage in pure bcc Fe and FeCr alloys, including the presence of impurities such as He, from molecular dynamics simulations

M. J. Caturla

University of Alicante
Spain

One of the objectives of this work is to study the damage production due to irradiation of pure Fe and Fe based alloys during the first few picoseconds using molecular dynamics simulations. And to then study the evolution of these defects to longer time scales using object kinetic Monte Carlo methods. We are interested in simulating two different experimental conditions: neutron irradiation and ion implantation. For that, we will study damage production in the bulk using periodic boundary conditions in our molecular dynamics simulations, and in thin films, considering films with the same thickness as those used in in situ TEM observations of ion implantation. The outcome of these calculations is a database of cascade damage for these materials during the first few picoseconds of irradiation as well as an understanding of the differences between the damage produced in bulk and thin films.

The work to be performed during the four years of the CRP is as follows:

During the first year we will study the damage produced in bcc Fe by recoils of energies between 50 and 100 keV. Results for bulk cascades as well as thin films will be obtained using molecular dynamics simulations. Calculations will be performed with two different interatomic potentials for Fe.

During the second year the calculations of the first year will be repeated in FeCr alloys for different Cr concentrations (between 2 and 12% Cr). Results of defect production (defect distribution, number and defect configurations) will be compared with those of pure Fe. Object kinetic Monte Carlo simulations of defect evolution to long time scales in the case of pure Fe will be also started during this second year.

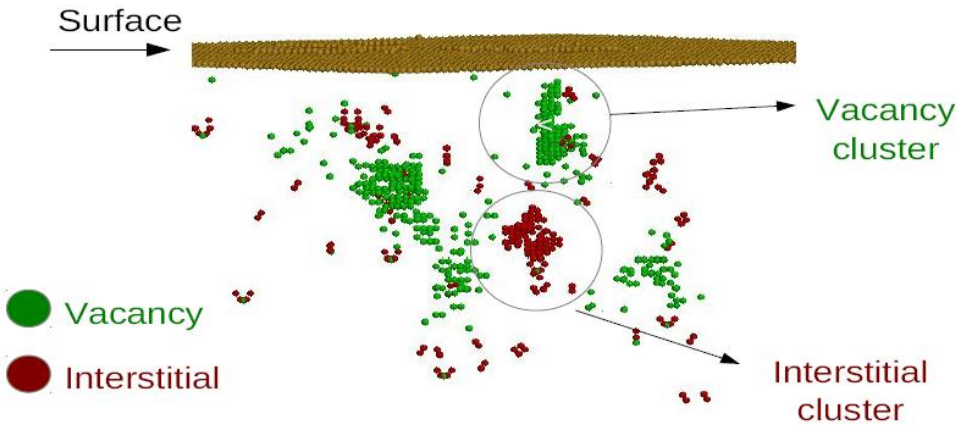
In the third year we will study the effect of impurities on defect production, particularly helium and carbon, using available interatomic potentials and comparing with the results of the first two years of the project.

In the fourth year we will finalize the research results and prepare the input for the CRP final document.

This work is part of the PhD thesis of María José Aliaga, from the University of Alicante.

During this year we have used the interatomic potential of Ackland and Mendelev [1] to compare with previous results obtained with the potential of Dudarev and P. Derlet [2]. These calculations have been performed varying the angle of incidence of the incoming ion, for 10^{o}, 22^{o} and 45^{o}, and energies of the ion of 50, 100 and 150 keV. The thin films have a thickness between 40 and 80 nm. Also, we have calculated the damage in the bulk material under the same conditions used for the thin films. The recoil energies used for the bulk simulations have been 50 and 100 keV. These calculations were performed at low temperature in order to isolate the effect of surfaces from the effect of defect migration. To account for the effect of temperature we have started calculations at 300K both in the bulk and in the thin films. In each condition several simulations were run to obtain statistically meaningful results. We have quantified the damage obtained with the two potentials and for the bulk calculations in terms of number of clusters and cluster size distribution.

The main scientific result is that the damage in thin films is significantly different to that in the bulk. When an ion deposits its energy close to the front or the back surface large vacancy loops and surface damage are created. The figure shows the last configuration of defects produced by a 50 keV Fe ion for the case of the AM potential [1]. In this picture the red dots are the locations of interstitial atoms, the green dots are vacancies. The yellow dots represent the surface and the adsorbed atoms above it. Large (> 1 nm) vacancy and self-interstitial clusters are observed in this particular cascade. In addition, this work could explain in-situ TEM experiments of ion implanted samples where vacancy loops have been identify in thin regions for low doses [3].



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TALYS, TENDL and Total Monte Carlo for primary irradiation damage

A.J. Koning and D. Rochman
NRG Petten
The Netherlands

Introduction

According to this summary report, NRG's TENDL library and its related uncertainty method, Total Monte Carlo (TMC), is now used by various parties in this CRP on primary radiation damage:

- KIT (Konobeyev and Fischer): comparison of TENDL recoils with other nuclear data libraries and gas production
- Sandia (Griffin): TENDL and TMC for displacement KERMA and damage energy in electronics
- CEA Saclay (Luneville, Crocombette and Simeone): damage energy calculations with DART using TENDL
- CCFE (Sublet and Gilbert): DPA calculations with FISPACT-II using TENDL
- UPM (Cabellos): TENDL and TMC for calculation of damage and its uncertainties
- NRG (Koning and Rochman): Maintenance and development of TENDL and TMC, specific for damage calculations

and hopefully other the CRP partners using nuclear data libraries will also consider TENDL as an option in their future work.

The results are mixed, which is not that strange since it is the first time that nuclear data libraries are consistently used on such a broad basis, and by independent parties, for damage calculations. Our main objective is to critically examine the applied analyses by others performed in this CRP, and to react to that with yearly improved versions of TENDL. As far as we know, this is the only initiative in the world where nuclear data needed for damage calculations are provided on a consistent basis. It requires:

- nuclear data for all isotopes that could be of relevance for irradiation damage
- inclusion of recoil information for all relevant channels
- inclusion of all particle production channels (especially protons and helium)
- extension beyond the traditional 20 MeV limit
- provision of uncertainty data that is processable for damage calculations

Below we will argue that the TENDL + TMC combination does just that.

TENDL

We will briefly discuss the latest version of the TALYS Evaluated Nuclear Data Library, TENDL, which is released around the time of this writing. This TENDL-2013 library contains sub-libraries for incident neutrons, protons, deuterons, tritons, helium-3's, alphas, and photons. For all types of incident particle, nuclear data libraries for 2626 nuclides are produced. These are all isotopes, in either ground or metastable state, with a half-life longer than 1 sec from Z = 3 (Li) to Z = 110 (Ds). This is about 8 times more nuclides than in any other world library. All libraries extend up to 200 MeV, contain covariance information, and are as complete as the ENDF format allows it to be. Table 1 compares TENDL with the other world libraries for some quantities relevant for this CRP.

Since its first version, TENDL-2008, it has been our aim to yearly produce nuclear data libraries which are complete from the nuclear reaction point of view. In ENDF language, this means a full nuclear reaction description from MF1 to MF40. Hence, every isotopic evaluation contains *all* possible nuclear reaction information, whether relevant for a particular application or not. The main challenge of the TENDL team now is to choose each year the right priorities for successive improvement, which obviously depends on many things, one of them being funding. Improvements could be better integral performance of criticality and reactor benchmarks, better overlap with differential data (EXFOR), more credible uncertainty information or, as relevant for this CRP, better

description of particle production and recoil channels and proper streamlining of the related ENDF-6 formatting issues.

At the basis of this evaluation system is the TALYS nuclear model code, which produces nearly all these data. Only for fission quantities and resonance parameters other software is used, see Fig. 1. A statistics code, TASMAN, performing among others a Monte Carlo sampling loop around the entire system, produces uncertainty information. The ENDF formatting code TEFAL, rivalling in programming complexity with TALYS, produces the nuclear data libraries. A full description of the system is given in [Kon12].

Table 1: Completeness of TENDL with emphasis on damage, compared to other world libraries

Library	# isotopes	# isotopes with recoils	# isotopes above 20 MeV
TENDL-2013	2626	2626	2626
ENDFB-VII.1	423	121	47
JENDL-4.0	405	5	0 (separate JENDLHE file)
JEFF-3.1.2	381	65	34

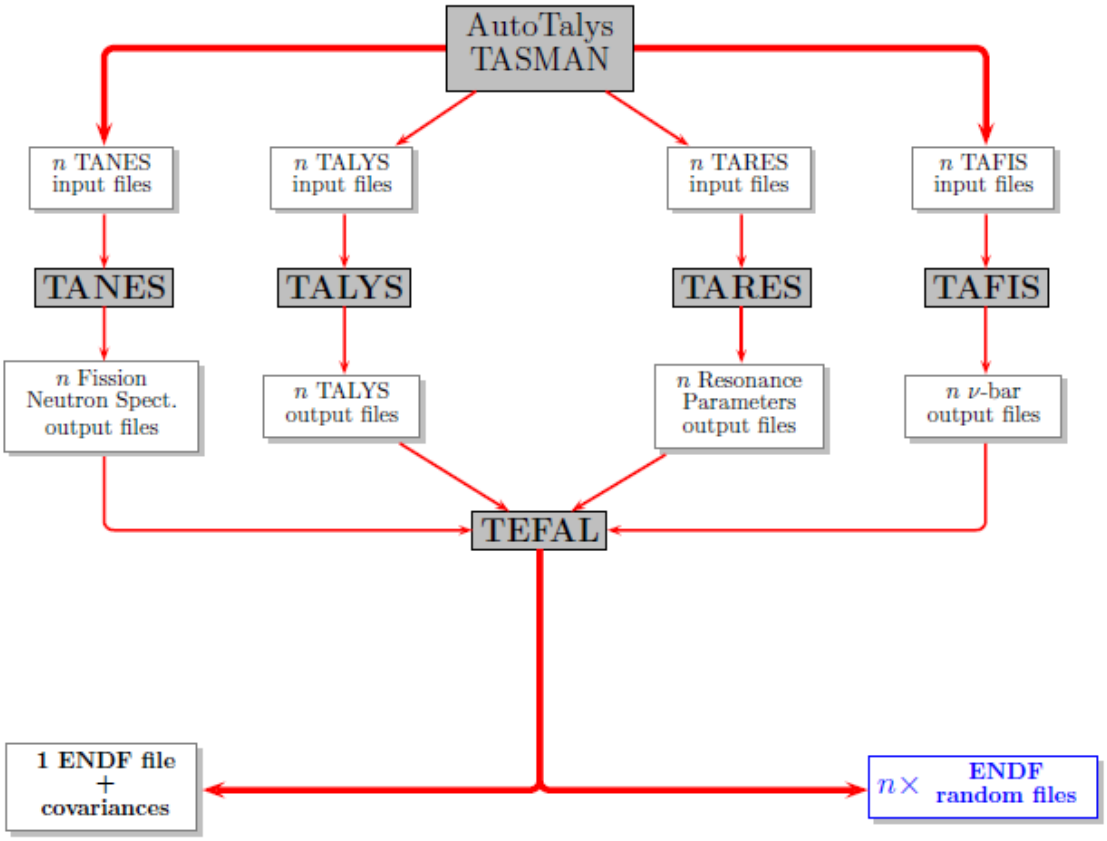

Figure 1. Flowchart of the nuclear data file evaluation and production process with the TALYS system.

Total Monte Carlo

For the TENDL library described above, a single ENDF-6 covariance data file is created by averaging the hundreds of random nuclear data sets coming from TALYS or other codes, see the box at the lower left hand side of Fig. 1. An alternative approach [Kon08] is to take the effect of a single random sampling of nuclear model parameters all the way to the end, i.e. to create one ENDF-6 file per random set of input parameters, process it and perform an applied calculation. This process is depicted in Fig. 2. In other words, every random curve is stored in a different ENDF-6 file, while every ENDF-6 file is complete for all quantities, i.e. MF1-15 are used. This approach has later been coined (by M. Herman) "Total" Monte Carlo (TMC) and makes uncertainty propagation a lot easier (apart from

the calculation time), and arguably more exact, than when using perturbation and covariance software. Covariance matrices simply do not appear in the entire process, with the exception of the extreme beginning, in the form of uncertainties and correlations of (model and experimental) input parameters, and the extreme end, e.g. an *average* DPA parameter, its uncertainty and covariance.

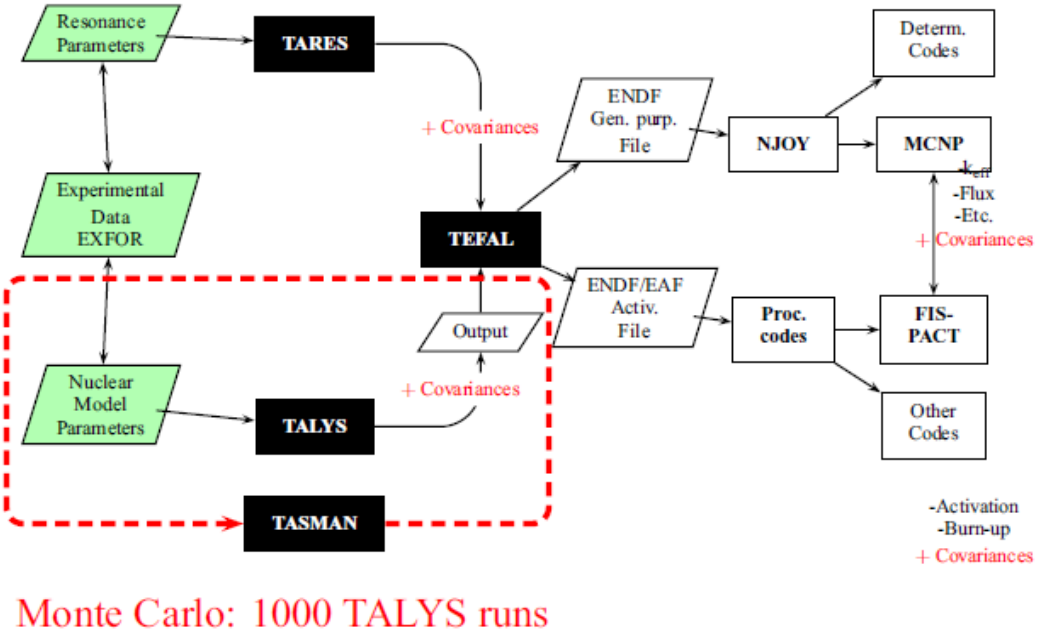

Figure 2: Flowchart of automated, reproducible evaluation process used for TMC and the production of TENDL.

Conclusions

Philosophers and (quantum)scientists sometimes debate the statement "If we cannot measure something then it does not exist". In nuclear data, until recently it used to be as if the statement "If we have not measured something, it is not relevant" applied. The quality of an isotopic evaluation is often *only* judged through comparison of existing experimental data, differential or integral. This means that the leading argument to adopt a certain isotopic evaluation over the other for any of the world libraries is probably *not* the existence of secondary reaction information (particle production, recoils etc.) that enables doing damage analyses. From the point of view of the maintenance method of these libraries (attempting to collect the best from many different contributing institutes) this is understandable. It does however lead to the statistics summarized in Table 1. The TENDL approach gets rid of that problem. TENDL-2012 was nearly complete, and TENDL-2013 is fully complete, in terms of reaction description. From now on it is zeroing in on the truth using differential and integral experimental data, and solving remaining glitches.

An important example of such a glitch is that at higher energies ia discontinuity at 30 MeV showed up in the NJOY damage curves calculated with TENDL-2011 and TENDL-2012. This was due to erroneous residual production cross sections in certain cases and a discontinuity in the center of mass frame for which the data were tabulated. The problem is now gone [Kon13], at least for the individual cases for which we checked this. In the timespan of this CRP, we will try to get the TENDL at a level where such deficiencies are gone.

References

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[Kon12] A.J. Koning and D. Rochman, "Modern nuclear data evaluation with the TALYS code system", Nucl. Data Sheets 113, 2841 (2012).

[Kon13] Private communication with B. MacFarlane, S. Kahler, O. Cabellos and J.C. Sublet.

Calculation of primary radiation damage parameters using ENDF/B-VII: Recoil spectra and damage cross sections

J. Kwon

Nuclear Materials Division
Korea Atomic Energy Research Institute (KAERI)
Korea

The overall objective of the proposed research is to generate primary radiation damage parameters for iron which include recoil atom spectra and damage cross sections. In the first year, the research activities of KAERI were focused on the molecular dynamics (MD) simulations of displacement cascade in iron, as well as the generation of the microscopic nuclear cross sections from the ENDF/B library. As a result of high-energy neutron interaction with materials, primary knock-on atoms (PKAs) are created in a direct or indirect way. The energy spectra of PKAs are dependent on such factors as the incident neutron energy, target atoms and the angle between the incident neutron and the recoil direction. According to the SPECTER code calculation, the energy of PKAs is distributed over a wide range from several eV to MeV. It is, therefore, necessary to calculate the damage parameters related to PKAs and accumulate that information systematically. PKAs can be generated by various nuclear reactions, including elastic/inelastic scattering and absorption reactions with neutrons. It is very important to estimate the probability of the occurrence of nuclear reactions with accuracy. In this research, we used the NJOY99 code system that can access directly the cross section and energy transfer data available in the ENDF/B-VII.

MD simulation of displacement cascades in iron

Simulations of displacement cascades were carried out with the MOLDY code, which has been used widely for MD calculations for bcc pure metals. The classical equations of motion for atoms are integrated via a Gear 4-value predictor-corrector algorithm and the many-body interatomic potential for α-iron, derived by Finnis and Sinclair, is embedded in the MOLDY. For a given value of PKA energy, we performed MD calculations with different positions and initial PKA directions. We used two PKA energies of 5 and 35 keV for cascade simulations; the former value corresponds to the average PKA energy of iron atoms in the light water reactor environments and the latter represents the average energy in the sodium-fast reactor environments. The cascade simulations have been performed until the recombination of interstitial and vacancy is finished. However, the atomic block does not return to a complete thermal equilibrium after the recombination phase due to a high temperature. Accordingly, we run the code until the number of point defects becomes stable.

The size distribution of the residual point defects is calculated from the MOLDY output by averaging the six simulation results. The distribution of defect clusters – interstitial and vacancy are plotted in Figure 1. The similar trends in clustering statistics could be observed for both conditions. In case of the high-PKA energy simulation, relatively larger clusters are found. The clustering formation of the interstitials is important in that these defects are thermally stable and can migrate away in groups from the parent cascade region to be absorbed at sinks.

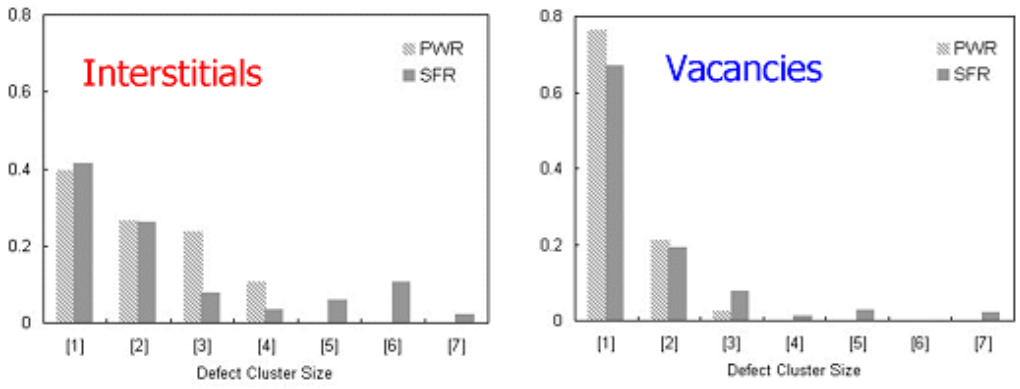

Figure 1. Size distribution of residual point defects for (a) interstitial and (b) vacancy; results of MD simulations, E_p= 5.2 keV for PWR and E_p = 35 keV for SFR (E_p= initial PKA energy).

Generation of microscopic cross sections from ENDF/B-VII

In quantifying the primary radiation damage due to neutron irradiation, the basic parameter is the displacement cross sections. The displacement cross section σ_d, can be defined as:

$$\sigma_d(E) = \sum_i \sigma_i(E) \int_{T_{min}}^{T_{max}} f_i(E,T) \cdot \nu_{NRT}(T)\ dT$$

where E is the incident neutron energy, T the energy of recoil, $\sigma_i(E)$ the nuclear cross section for i-type interaction at neutron energy of E, $f_i(E,T)$ the neutron-atom energy transfer kernel, T_{min} and T_{max} are the lower and upper energy of a recoil atom, respectively and are determined by the type of interaction of interest, and $\nu_{NRT}(T)$ represents the secondary displacement function calculated using the Norgett, Robinson, and Torrens modification of the Kinchin-Pease formula. Among several parameters composed of σ_d, the nuclear cross sections σ_i can be obtained from the previous ENDF/B libraries. Although the SPECTER code is very fast and simple, it has a shortcoming that latest nuclear data cannot be used since the older version of ENDF libraries are embedded in the code. Accordingly, we determined the use of the latest version of ENDF libraries through the NJOY99 code system. Ultimately we will calculate σ_d by combining the energy transfer kernel, which is available from the ENDF/B-VII. Figure 2 shows the microscopic cross sections for ^{56}Fe, which was plotted from the processing of NJOY-99.

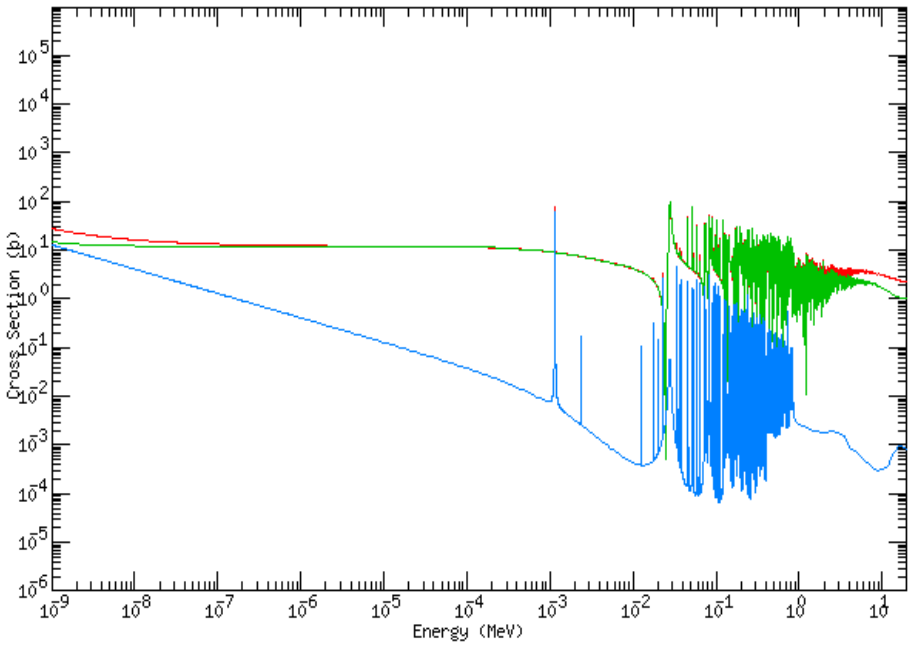

Figure 2. Microscopic cross sections for total (red), elastic scattering (green) and radiative capture (blue) reactions, process from the NJOY99 code system.

Year 1 (On going)

- Perform MD simulation of displacement cascade in iron (PKA energy: up to tens of keV)
- Generate microscopic nuclear cross sections from ENDF/B-VII using NJOY-99
- Calculate energy transfer kernel for each nuclear reaction

Year 2 (Plan)

- Build database for the results of displacement cascade simulation, including primary damage parameters of the cascade efficiency and cluster formation
- Develop an original computational code for generating recoil atom spectra

First Research Coordination Meeting (RCM-1) of CRP

"Primary Radiation Damage Cross Sections"

4 - 8 November 2013
IAEA Headquarters, Vienna, Austria
Meeting Room A 0742

AGENDA

(presentations's time is approximate and includes questions and breaks)

Monday, 4 November

09:30 - 10:15 **Opening**
Welcome address – **Meera Venkatesh** (NAPC, Director)
Self-introduction of Participants - **All**
Election of Chairperson and Rapporteur - **All**
Approval of Agenda - **All**
Administrative announcements – **Alexander Oechs** (NDS)

10:15 - 10:30 **Stanislav Simakov, NDS** - Objectives of CRP and its 1st RCM

10:30 - 11:00 **Dieter Leichtle, F4E** - Nuclear data for fusion applications: dpa beyond NRT?

Session 1: Presentations of Research Proposals

11:00 - 12:00 **Kai Nordlund, Uni Helsinki** - Summary of the final report of the OECD primary damage group

12:00 - 14:00 *Lunch break + Administrative issues*

14:00 – 15:00 **Larry Greenwood, PNNL** - The SPECTER computer code, describing the history, uses and limitations of the software

15:00 - 16:00 **Alexander Konobeyev, KIT** - Evaluation of displacement and gas production cross-sections for structure materials using advanced simulation methods and experimental data

16:00 - 17:00 **Yosuke Iwamoto, JAEA** - Calculation of PKA and DPA using event generator mode in PHITS code

Coffee breaks as needed

Tuesday, 05 November

9:00 – 10:00 **Liu Ping, CIAE** - The calculation method of KERMA and DPA in CNDC

10:00 – 11:00 **Patrick Griffin, SNL** - Uncertainty Analysis of Metrics Used for Assessing Primary Radiation Damage

11:00 – 12:00	**David Simeone, CEA**	- The interest of dpa to handle the microstructure of irradiated materials
12:00 - 13:00	**Oscar Cabellos, UPM**	- Processing of a damage energy cross-section library based on JEFF3.1.1 and the potential impact of nuclear data uncertainties on damage energy and gas production cross-sections
13:00 - 14:00	*Lunch break*	
14:00 - 15:00	**Skip Kahler, LANL**	- Using NJOY to Calculate 'Damage' with Modern Evaluated Nuclear Data Files
15:00 - 16:00	**Jean-Christophe Sublet, CCFE**	- Radiation damage: beyond dpa - from nuclear data to ....?
16:00 - 17:00	**Mark Gilbert, CCFE**	- Radiation damage: beyond dpa - visualisation techniques
17:00 - 18:00	**Roger Stoller, ORNL**	- Details of cascade damage production relevant to damage accumulation

Coffee breaks as needed

Wednesday, 06 November

9:00 - 10:00	**Chung Woo, Uni Hong Kong**	- Correlated Point-Defect Production from Cascades
10:00 - 11:00	**Dmitry Terentyev, SCK-CEN**	- Development of potentials to study primary damage effects in Fe-Ni-Cu-Mn system
11:00 - 12:00	**Fernando Mota, CIEMAT**	- Beyond NRT concept: using BCA codes to design irradiation experiments to emulate neutron fusion effects in materials
12:00 - 13:00	**Ivan Bondarenko, IPPE**	- The improvement of the (n,α) reaction investigation method and first preliminary results
13:00 - 14:00	*Lunch break*	
14:00 - 17:00	**Session 2: Discussion of expected outputs, individual contributions and their coordination**	

Coffee breaks as needed

19:00 - ***Hospitality event in*** *Restaurant "**Gösser Bierklinik**"* *http://www.goesser-bierklinik.at/*

Thursday, 07 November

09:00 - 12:30	**Session 2: Discussion of expected outputs, individual contributions and their coordination**
12:30 - 14:00	*Lunch break*
14:00 - 18:00	**Session 2: Drafting of the Summary Report of the Meeting**

Coffee breaks as needed

Friday, 08 November

09:00 - 12:30	**Session 2: Review of the Meeting Summary Report**
≈ 15:00	***Closing of the Meeting***

1st Research Coordination Meeting of the CRP
"Primary Radiation Damage Cross-Sections"

4-8 November 2013
VIC A0742, Vienna, Austria

LIST OF PARTICIPANTS

BELGIUM Mr Dmitry Terentyev Centre d' Etude de l'Energie Nucleaire Boeretang 200 2400 Mol Tel.: +32 14 33 31 97 E-mail: dterenty@sckcen.be	**FRANCE** Mr David Simeone CEA Saclay DEN/DANS/SRMA/LA2M Bat 453 – Pce 27B 91191 Gif-sur-Yvette Tel.: +33 1 69 08 29 20 E-mail: david.simeone@cea.fr
CHINA Mr Chung Ho Woo The City University of Hong Kong College of Science and Engineering The Chee Avenue Hong Kong SAR Tel.: +852 3442 7848 E-mail: chungwoo@cityu.edu.hk	**FRANCE** Mr Laurence Luneville CEA Saclay DEN/DANS/SRMA/LA2M Bat 453 – Pce 27B 91191 Gif-sur-Yvette Tel.: E-mail: Laurence.luneville@cea.fr
CHINA Ms Liu Ping China Nuclear Data Center China Institute of Atomic Energy P.O. Box 275 (41) Beijing Tel.: + 86 10 6935 7712 E-mail: ping@ciae.ac.cn	**GERMANY** Mr Alexandre Konobeev Institute for Neutron Physics and Reactor Technology Karlsruhe Institute of Technology Herman von Heimholtz Platz 1 76344 Eggenstein-Leopoldshafen Tel.: +49 721 608 23768 E-mail: alexander.konobeev@kit.edu
FINLAND Mr Kai Nordlund Department of Physics University of Helsinki P.O. Box 43 Pietari Kalmink. 2 00014 Helsinki Tel.: +358 9 19150007 E-mail: kai.nordlund@helsinki.fi	**GERMANY** Mr Ulrich Fischer Institute for Neutron Physics and Reactor Technology Karlsruhe Institute of Technology Herman von Heimholtz Platz 1 76344 Eggenstein-Leopoldshafen Tel.: +49 721 608 23407 E-mail: Ulrich.fischer@kit.edu

JAPAN Mr Yosuke Iwamoto Japan Atomic Energy Agency 2-4 Shirakata-shirane Ibaraki-ken, Nakagun Tokaimura 319-1194 Tel.: +029 282 5195 E-mail: iwamoto.yosuke@jaea.go.jp	**SPAIN** Mr Dieter Leichtle ITER Department Fusion for Energy c/ Josep Pla, n° 2 Barcelona 08019 Tel.: +34 93 489 7459 E-mail: dieter.leichtle@f4e.europa.eu
KOREA, Republic of Mr Junhyun Kwon Korea Atomic Energy Res. Institute (KAERI) 1045 Daedeok-Daero Yuseong-gu Daejeon 305-353 Tel.: +82 42 868 8588 E-mail: jhkwon@kaeri.re.kr	**SPAIN** Ms Maria Caturla Universidad de Alicante Carretera San Vicente del Raspeig s/n San Vicente Alicante Tel.: +34 965 903400 E-mail: mj.caturla@ua.es
NETHERLANDS Mr Arjan Koning Nuclear Research and Consultancy Group (NRG) Westerduinweg 3 P.O. Box 25 1755 ZG Petten Tel.: +31 22456-4051 E-mail: koning@nrg.eu	**SPAIN** Mr Rafael Vila Fusion National Laboratory CIEMAT Avenida Complutense 40 28040 Madrid Tel.: +34 91 3466580 E-mail: Rafael.vila@ciemat.es
RUSSIA Mr Ivan Bondarenko Institute for Physics and Power Engineering Bondarenko Ploshad 1 Obninsk Tel.: E-mail: ibondarenko@ippe.ru	**UNITED KINGDOM** Mr Jean-Christophe Sublet UK Atomic Energy Authority Culham Centre for Fusion Energy Abingdon Oxfordshire OX14 3DB Tel.: +44 1235 466400 E-mail: jean-christophe.sublet@ccfe.ac.uk
SPAIN Mr Fernando Mota Laboratorio National de Fusion Avenida Complutense 40 CIEMAT 28040 Madrid Tel.: +34 91 346 6578 E-mail: Fernando.mota@ciemat.es	**UNITED KINGDOM** Mr Mark Gilbert UK Atomic Energy Authority Culham Centre for Fusion Energy Abingdon Oxfordshire OX14 3DB Tel.: E-mail: mark.gilbert@ccfe.ac.uk
SPAIN Mr Oscar Cabellos Universidad Politecnica de Madrid C/Ramiro de Maeztu 28040 Madrid Tel.: E-mail: Oscar.cabellos@upm.es	**UNITED STATES OF AMERICA** Mr Roger Stoller Oak Ridge National Laboratory P.O. Box 2008, MS 6114 Oak Ridge TN 37831-6114 Tel.: +1 865 576 7886 E-mail: rkn@ornl.gov; stollerre@ornl.gov

UNITED STATES OF AMERICA Mr Patrick Griffin Sandia National Laboratories P.O. Box 5820 Albuquerque NM 87185 Tel.: +1 505 845 9121 E-mail: pjgriff@sandia.gov	**IAEA** Mr Stanislav Simakov Scientific Secretary Head, Nuclear Data Services Unit Nuclear Data Section Division of Physical and Chemical Sciences Tel.: +43 1 2600 21717 E-mail: s.simakov@iaea.org
UNITED STATES OF AMERICA Mr Albert C. (Skip) Kahler III Los Alamos National Laboratory Building 200, Room 215 P.O. Box 1663, MS B214 Los Alamos NM 87545 Tel.: +1 505 606 2042 E-mail: akahler@lanl.gov	**IAEA** Mr Robin Forrest Head, Nuclear Data Section Division of Physical and Chemical Sciences Tel.: +43 1 2600 21709 E-mail: r.forrest@iaea.org
UNITED STATES OF AMERICA **CONSULTANT** Mr Lawrence R. Greenwood Pacific Northwest Laboratory MS P7-22, P.O. Box 999 Richland WA 99352 Tel.: +1 509 375 5301 E-mail: Larry.Greenwood@PNL.GOV	**IAEA** Mr Naohiko Otsuka Nuclear Data Services Unit Nuclear Data Section Division of Physical and Chemical Sciences Tel.: +43 1 2600 21715 E-mail: n.otsuka@iaea.org
	IAEA Ms Valentina Semkova Nuclear Data Services Unit Nuclear Data Section Division of Physical and Chemical Sciences Tel.: +43 1 2600 21727 E-mail: v.semkova@iaea.org

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://www-nds.iaea.org