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The use of the SRIM code for calculation of radiation damage induced by neutrons

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ABSTRACT

Materials subjected to neutron irradiation will being evolve to structural changes by the displacement cascades initiated by nuclear reaction. This study discusses a methodology to compute primary knock-on atoms or PKAs information that lead to radiation damage. A program AMTRACK has been developed for assessing of the PKAs information. This software determines the specifications of recoil atoms (using PTRAC card of MCNPX code) and also the kinematics of interactions. The deterministic method was used for verification of the results of (MCNPX+AMTRACK). The SRIM (formely TRIM) code is capable to compute neutron radiation damage. The PKAs information was extracted by AMTRACK program, which can be used as an input of SRIM codes for systematic analysis of primary radiation damage. Then the Bushehr Nuclear Power Plant (BNPP) radiation damage on reactor pressure vessel is calculated.

1. Introduction

Irradiation of materials with particles that are energetic enough to create atomic displacements could easily induce radiation damages in materials. As a result of neutron irradiation, the produced defects on the lattice structure affect the mechanical, electrical and other physical properties of irradiated materials. The spatial configuration of the damage produced by bombarding particles depend mainly on the projectile type and its energy, which results in differences in defect clustering, swelling, growth, phase change, segregation, bubble formation and dissolution rate. All these features directly cause to the microstructural evolution of materials [1].

The first step in assessing radiation effects is to create a primary knock-on atom or PKA by a nuclear reaction, a radioactive decay, scattering of incident radiation or injection from an accelerated ion beam. The effects of neutron irradiation on structural materials of a nuclear reactor depend on the neutron spectra and the time of irradiation. If we would like to compare affected materials in different type of facilities, then we have to consider an exposure parameter that takes into account the differences in the neutron spectrum. The effects of these spectral differences have been accounted through the displacements per atom (dpa) index, which is known as a calculated representation of the number of primary and secondary atoms that are displaced from their lattice sites due to neutron irradiation. It is necessary to review some topics mainly from nuclear physics, such as radioactive decay, nuclear reactions and the neutron scattering of nuclei, to understand the quality of production of primary recoils [2–4]. Several approaches exist for predicting and calculating the formation, evolution and behavior of radiation damages, including: the binary collision approximation (BCA) method, the molecular dynamics (MD) method and the kinetic Monte Carlo (KMC) method. All of these techniques require data, as input at some level, about the initial events in the form of the type, energy and spatial distribution of the PKAs [5,6].

In this work the MCNP version X was used which has an extended capability for solving neutron, gamma and electron problems in a complex and three dimensional geometries and also the standard cross section libraries are included [7]. Different outputs of MCNPX qualify this code to be applicable in different calculations in reactor physics and also radiation damage [8].

The other well-known code is used to calculate the damage cascades in a target is SRIM code [9–12]. It uses the file Trim.dat as input which contains the kinetic information about atoms which start recoil cascades.

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In this work the code is written by MATLAB software. MATLAB is a professional mathematical software which is applied for mathematical algorithms development and data visualization and analysis. The code named AMTRACK, which reads the output from MCNPX with PTRAC card and uses it as input for SRIM, has been designed to calculate the neutron radiation damage. The file Trim.dat is generated by combination of two powerful programs (MATLAB program and MCNPX code) which extract the PKAs information. Then SRIM takes AMTRACK output information and calculates the target damage.

Most modeling of neutron induced displacement damage has been focused on reactor structural materials, especially stainless steel that mainly composed of iron, nickel and chromium [2,13]. The present work is devoted to calculation of the primary knock-on atoms spectrum in these elements that irradiated with neutrons of PWR reactors. In the older papers for calculation of primary recoil spectra used a computer code such as SPECTER [14], DART [15], PHITS [16] or deterministic methods that solved a deterministic integral [2]. Because of the importance of these analytic formulations, prediction of PKA spectrum by using detailed Monte Carlo modeling (AMTRACK) are compared with prediction of PKA spectrum made using deterministic method. The information that required for SRIM input (initial ion energy, trajectory and starting position) is acquired by using AMTRACK program. Finally, the advantages of using AMTRACK program are discussed.

2. Material and methods

There are two different mechanisms that displace atoms from their lattice position in a material irradiated with neutrons. The first mechanism is elastic and inelastic collisions between neutrons and nuclei where the target receives a strike from the incident particle and would be able to produce further displacements before being decelerated to rest in the lattice and finally the target nucleus in this process remains unchanged.

The second mechanism of atomic displacement is caused by neutron capture interaction and subsequent nuclear reactions. The target nucleus in this reaction may undergo fission, gamma emission or production of charged particle like hydrogen or helium which may cause atomic displacements. If target has adequately high neutron capture cross section for low energy neutrons and the reaction is exothermic, atomic displacement may be created even by thermal neutrons which do not have sufficient energy to produce damage in direct reactions [2]. Because of very high cross section of elastic and inelastic scattering in comparison with other reactions such as $(n, p)(n, \alpha)(n, n\alpha)(n, 2n)$, in this work we restrict our calculation to elastic and inelastic scattering and neglect the other reactions that produce atomic displacement. The validity of neglecting other reactions is shown in Figs. 1, 2, 3 that acquired by JANIS software. JANIS is a visual program prepared to facilitate the manipulation and visualization of nuclear data. The objective of this program is to assessment of numerical data and graphical representations by the users. It is completely flexible program for different nuclear data sets comparison [17]. The PWR spectrum weighted cross section for neutron interactions (elastic, inelastic, capture and alpha production) as a function of neutron energy for ^{56}Fe, ^{58}Ni, ^{52}Cr are plotted in Figs. 1, 2 and 3. These approximations are reasonable at energies 1 eV to a few MeV for iron, nickel and chromium elements.

2.1. Monte-Carlo simulations

In order to calculate displacements per atom (dpa) resulting from neutrons, we suggest to use SRIM code. SRIM requires as input the types, energies, initial positions and direction cosines

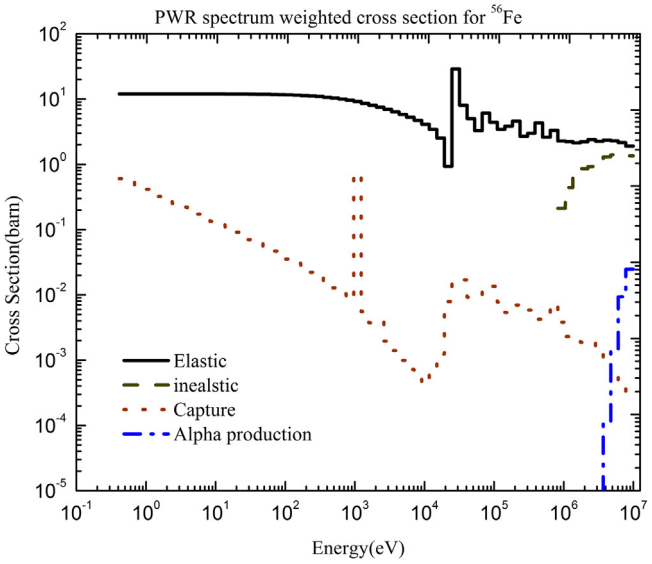

Fig. 1. Nuclear reactions cross section (barn) for taken from ENDF/B-VII.1 **(17)** and weighed by Janis software **(16)** iron.

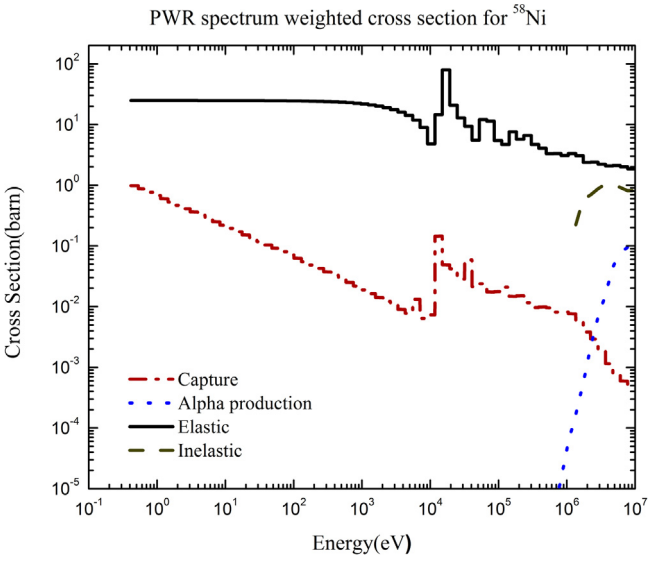

Fig. 2. Nuclear reactions cross section (barn) for taken from ENDF/B-VII.1 **(17)** and weighed by Janis software **(16)** nickel.

of the PKAs. These input parameters were received by modeling the transport of neutrons through the material with MCNPX. The PTRAC option of MCNPX code registers the whole history, such as interaction type, energy, direction and position of particle through MCNPX run. The Ptrac file is completely described in Appendix I from the MCNPX manual [7].

A MATLAB program, called AMTRACK, was written to determine the specifications of PKAs using the kinematics of interaction and the Ptrac output, produces an input for SRIM code, and however for explanation of operations performed within the system the flowchart of AMTRACK program is shown in Chart 1.

AMTRACK was written to extract neutron characteristics (energy, position, and direction cosines), before and after each collision then based on conservation of energy and momentum, the PKA characteristics (atomic species, energy, position, and direction cosines), were determined for elastic and inelastic collisions.