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Primary knock on atom spectra, gas production and displacement cross section for tungsten and chromium irradiated with neutrons at energies up to 14.1 MeV

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ABSTRACT

In the ITER and other proposed fusion reactors, chromium and tungsten are proposed as first wall materials. Fusion of DT plasma will produce neutrons of 14.1 MeV energy. Nuclear reactions of fusion reactor material with such high energy neutrons lead to the displacement cascades and gas production in the reactor materials. All probable reaction channels such as (n,n'), (n,2n), (n,p), (n,α) and (n,d) are open for the interactions of these neutrons with tungsten and chromium. In the present study, energy spectra of recoils or PKA, gas production and displacement cross section for tungsten and chromium at neutrons of up to 14.1 MeV energy have been predicted using the appropriate nuclear models in the TALYS-1.8 code. In the cross section and PKA calculations, the contributions from possible reaction mechanisms such as direct, pre-equilibrium, and compound nuclear mechanisms have been considered. Calculated energy spectra of protons, alpha particles, and outgoing neutrons have been compared with recent ENDF-VIII, JEFF-3.3 and TENDL-2017 data libraries and discrepancies among them have been discussed. PKA data from each reaction channels have been calculated. PKA data have been used to predict the displacement cross-section with the Norgett, Robinson, and Torrens (NRT) approach. Calculated displacement cross section data of chromium and tungsten have been compared with existing data.

1. Introduction

The quantification of displacement per atom (DPA), gas production per atom (GPA) and nuclear heating in the fusion reactor materials are essential to ensure the reliable functioning and structural integrity of fusion reactor components. Damage (quantized by DPA) and gas production can decrease the lifetime and strength of the reactor components, respectively. Tungsten will be used as the divertor material in ITER machine and also has been proposed for upcoming fusion devices in the plasma facing materials [1]. This is due to its high thermal conductivity of 1.75 W cm^{-1} K^{-1}, high melting point of 3422 °C, and high threshold of 216 eV for deuterium ion sputtering [2]. The other functional materials that will be used in fusion reactors are chromium and copper alloys [3]. Chromium is one of the major constituents of stainless steel (SS). SS is an important structural material to be used in the vacuum vessel and shield modules of ITER machine. CuZrCr alloy is proposed to be used in the first wall, blanket, and divertor in ITER machine to enhance the heat removal capability [3].

Materials in ITER and other proposed fusion devices have to endure the high flux of 10^{15} neutron/cm^2/sec of up to 14.1 MeV energy. All the probable reaction channels such as (n,n'), (n,2n), (n,p), (n,α), (n,d) and (n,gamma) are viable for neutrons of this energy range in the reactor materials. Nuclear reaction channels such as (n,p), (n,np), (n,α) and (n,nα) yield hydrogen and helium gases in the reactor materials. Therefore, reaction cross-section data of these reaction channels need to be evaluated for quantifying the gas production inside the reactor materials. Reaction channels such as (n,el), (n,2n), (n,p), (n,α) and (n,gamma) yield energetic ejectiles along with the recoil nucleus. Recoil nuclei from different reaction channels act as primary knock on atoms (PKA). The damages by PKA in the materials are due to the formation of dislocations, Frenkel pairs, crowdions, etc [4] and lead to the displacements in the atomic lattices of the reactor materials. Event by event analysis of the interactions of PKA with the surrounding lattice and calculation of displacement cross section (σ_{DPA}) by Norgett, Robinson and Torrens (NRT) method are the methods by which DPA is calculated. $\sigma_{DPA(NRT)}$ multiplied with the neutron fluence gives DPA_{NRT}. NRT method does not include recombination and relocation of defects in its calculations. DPA_{NRT} is used as the designing parameter to

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optimize the material suitability for fusion devices [4]. DPA_{NRT} has also been adopted as standard practices in the ASTM (American society for testing and materials) E693 and ASTM E521 [5]. In the both ASTM E693 and ASTM E521 technical reports, displacement of atoms are considered as the major source of neutron induced damage. In these technical reports, neutron induced displacement cross section had been produced with the NRT approach using the nuclear data from ENDF-VI data library. Event by event analysis can be carried out with binary collision approximation (BCA) method, molecular dynamics (MD) method, and kinetic Monte-Carlo method. Event by event analysis of PKA interactions is used to study the mobility of defects, recombination of vacancies, and clustering of interstitials. In both, NRT and event by event approach, energy spectra of PKA from all the open reaction channels are the essential data. PKA for all the reaction channels can be experimentally measured form the energy differential cross-section (EDX) data of ejectiles. Energy spectra of ejectiles and recoils are not available in the experimental data libraries for the most of the fusion related materials. Displacement cross section can be produced with the NJOY code [6]. NJOY code processes angle energy distribution data of ejectiles from ENDF data libraries and produces displacement cross-section with the NRT approach. In the present study, displacement cross section data have been calculated with the NRT method using the PKA data from TALYS code. Calculated displacement cross section is compared with the existing displacement cross section data which had been produced with the NJOY code using the ENDF and JEFF data libraries. Calculated data of EDX have also been compared with the evaluated data from up to date nuclear data libraries such as ENDF-VIII, TENDL-2017, JEFF-3.3 and discrepancies among them have been discussed.

In this present work, excitation functions of (n,n'), (n,2n), (n,p) and (n,α) reaction channels on ^{184}W, energy differential cross section (EDX) of charged particle emission reactions, PKA spectra of all the reaction channels, gas production and displacement cross section of tungsten and chromium have been reported for the neutrons of up to 14.1 MeV energy.

2. Methodology and calculation methods

In the present work, calculation of EDX data, recoil spectra, gas production cross section (σ_{GPA}) and displacement cross section ($\sigma_{DPA(NRT)}$) have been carried out in three steps and is as follows,

1) TALYS-1.8 code has been used to validate the nuclear models and parameters for the calculations of cross section data of tungsten and chromium. It was previously used by Avrigeanu et al. [7] to study the pre-equilibrium reaction mechanism of neutron induced reactions on the stable isotopes of tungsten. A. Trkov et al. [8] had also calculated neutron induced reaction cross section data for the stable isotopes of tungsten with Empire-2.1 code for ENDF-VIII data library. Similarly, P. Pereslavstev et al. [9] had also calculated nuclear data with GNASH code for stable isotopes of tungsten for the JEFF-3.2 and JEFF-3.3 data libraries [9]. Excitation functions of (n,el), (n,2n), (n,p) and (n,α) reaction channels for ^{184}W have been calculated with the TALYS-1.8 code. Appropriate nuclear models have been adopted by comparing the calculated reaction cross section data with the existing cross section data [10–17] from EXFOR Data library and evaluated data libraries [18–20]. For Chromium, nuclear models are adopted from Mayank et al. [21].
2) Adopted nuclear models are used in the calculations of EDX of charged particles and outgoing neutrons. The experimental EDX data of charged particles and outgoing neutrons for stable isotopes of tungsten are not available in experimental data libraries of IAEA (EXFOR). Many researchers had measured EDX data from double differential cross section (DDX) data of charged particles emission reactions [22–24] for other fusion reactor materials. Theoretical study of EDX of charged particles emission reactions on the stable isotopes of chromium had been carried out by Mayank et al. [21] and Demir et al. [25]. Mayank et al. [21] and Demir et al. [25] had used TALYS-1.6 code to predict the EDX and DDX data and compared the calculated results with the experimental data to validate nuclear models and parameters. TALYS code was also used to calculate the DDX data of charged particles from fusion related materials [26,27] at 14 MeV neutron energy. Energy spectra of PKA from all the open reaction channels have been calculated with the adopted nuclear models and parameters.
3) Displacement cross section has been calculated using the standard NRT method. σ_{DPA} of tungsten was calculated for the neutrons [28] and protons [29] of up to 1 GeV energy using the NJOY and IOTA code [30]. Broeders et al. [28,29] had produced displacement cross section data using the recoil spectra from ENDF-VI data library with the NJOY code. Broeders et al. had used the NRT and BCA-MD approach to calculate displacement cross sections. In the BCA + MD approach, successive interactions of PKA with target lattice, primary radiation defects (PRD) such as the formation of Frenkel pair, interstitial clusters, recombination and relocations of atoms have been taken into consideration. In BCA + MD method, PRD are simulated using the BCA and MD methods. NRT method does not incorporate PRD in its approach thus predicts displacement cross section higher than the BCA + MD approach. NRT approach was used by Iwamato et al. [31] and Chang et al. [32]. Iwamato et al. [31] had used PHITS code for the calculation of recoil spectra. KIT database of displacement cross section comprises the displacement cross section data of chromium which was calculated with the NJOY code using the nuclear reaction data from ENDF-VII.

Calculations of σ_{GPA} and σ_{DPA} have been carried out for all the stable isotopes of tungsten (^{180}W, ^{182}W, ^{184}W, ^{186}W, ^{183}W) and chromium (^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr).

2.1. Selection of nuclear models in TALYS code

For the neutrons of up to 14.1 MeV energy, total reaction rate comprises of pre-equilibrium and direct reaction along with the compound nuclear reaction mechanism. TALYS-1.8 [33] calculates nuclear reaction cross section data for different incident particles. It can produce nuclear reaction data as well as it can also be used to validate nuclear models. It can perform optical model, pre-equilibrium, direct and compound nuclear calculations for neutrons, photons, proton and alpha particles. It provides the usage of different nuclear models as well as the modified nuclear parameters into its calculations. It can calculate reaction, energy differential and double differential cross section data for neutron induced reactions of up to 200 MeV energy incident neutrons. Optical model potentials are derived from Konning et al. [34] in TALYS code for the optical model calculations. In its default mode, Compound nuclear calculations are carried out with Hauser Feshbach method [35] with the width fluctuation correction calculated by Molduer method, pre-equilibrium calculations are carried out with the exciton models [36] and level density parameters are calculated with Fermi temperature and gas model [37]. Direct and optical model calculations have been adopted from ECIS06 code [38]. ECIS06 code works on distorted wave born approximation (DWBA) method [39]. Apart from these models, many alternate nuclear models and parameters can be selected and revised.

For ^{184}W, Excitation functions of (n,el), (n,2n), (n,p) and (n,α) reaction channels have been evaluated for the neutrons of up to 14.1 MeV energy. Calculated data have been compared with the cross-section data available in the EXFOR data library. Based on the agreement with the experimental data, nuclear models are selected for the further calculations. Level density model of constant temperature and fermi gas model [40] predicts the best fitted cross section data for (n,p) reactions, Fermi back shifted model [40] predicts the best fitted data for (n,α) reactions. Level density parameters from Goriely's tables with the pure Hauser Feshbach model of compound nuclear calculations predict the