

New Data Files for the Calculation of Neutron and Proton Induced Radiation Damage Rates in Structural Materials of High Energy Systems

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Abstract

Displacement cross-sections were obtained for chromium, iron, and nickel using results of the molecular dynamics simulations and calculations using the binary collision approximation model at incident neutron and proton energies from 10^{-5} eV up to 1 GeV. The IOTA code was applied to obtain the number of defects in irradiated materials. At low energies of incident particles nuclear recoil spectra were calculated using ENDF/B-VII data and the NJOY code. Displacement cross-sections are stored using the ENDF-6 format. The first intended application of obtained cross-sections is the calculation of radiation damage dose for materials irradiated in MEGAPIE.

1. Introduction

The calculation of the radiation damage rate in structural materials using results of molecular dynamics simulations (MD) is one of the actual tasks of evaluating of the primary damage of structural materials irradiated in reactors and advanced nuclear energy systems. The first attempts to get displacement cross-sections usable for such calculations have been made for tantalum, tungsten, and iron in Refs.[1,2].

In the present work displacement cross-sections were obtained for chromium, iron, and nickel at the incident nucleon energies from 10^{-5} eV up to 1 GeV using the results of MD simulations and calculations using the binary collision approximation model (BCA). Data for proton irradiation of iron [2] were revised and improved.

The displacement cross-section is calculated as follows

$$\sigma_d(E_p) = \sum_i \int_{E_d}^{\infty} d\sigma(E_p, Z_T, A_T, Z_i, A_i, T_i) / dT_i \times v(T_i, Z_T, A_T, Z_i, A_i) dT_i \quad (1)$$

where E_p is the energy of the incident particle; $d\sigma/dT_i$ is the recoil atom energy distribution depending on Z_T , A_T , Z_i , and A_i which are atomic and mass numbers of the target and the recoil atom produced in the i -th reaction channel, correspondingly, for the elastic scattering $Z_i = Z_T$, $A_i = A_T$; $v(T_i)$ is the number of Frenkel pairs produced by the primary knock-on atom (PKA) with the kinetic energy T_i ; $T_i^{\max}$ is the maximal kinetic energy of the PKA produced in i -th reactions.

The number of defects produced in irradiated material is equal to

$$v(T_i) = \eta(T_i) N_{\text{NRT}}(T_i), \quad (2)$$

where η is the defect production "efficiency" [1,2] and N_{NRT} is the number of defects calculated according to the NRT model

$$N_{\text{NRT}} = 0.8 \cdot T_{\text{dam}} / (2E_d), \quad (3)$$

where T_{dam} is the energy transferred to lattice atoms in collision cascades reduced by the losses for electronic stopping of moving atoms; E_d is the effective threshold displacement energy.

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Table of Contents Neutron Data Of Structural Materials For

1. Understanding the eBook Neutron Data Of Structural Materials For
 - The Rise of Digital Reading Neutron Data Of Structural Materials For
 - Advantages of eBooks Over Traditional Books
2. Identifying Neutron Data Of Structural Materials For
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Neutron Data Of Structural Materials For
 - User-Friendly Interface
4. Exploring eBook Recommendations from Neutron Data Of Structural Materials For
 - Personalized Recommendations
 - Neutron Data Of Structural Materials For User Reviews and Ratings
 - Neutron Data Of Structural Materials For and Bestseller Lists

5. Accessing Neutron Data Of Structural Materials For Free and Paid eBooks
 - Neutron Data Of Structural Materials For Public Domain eBooks
 - Neutron Data Of Structural Materials For eBook Subscription Services
 - Neutron Data Of Structural Materials For Budget-Friendly Options
6. Navigating Neutron Data Of Structural Materials For eBook Formats
 - ePub, PDF, MOBI, and More
 - Neutron Data Of Structural Materials For Compatibility with Devices
 - Neutron Data Of Structural Materials For Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Neutron Data Of Structural Materials For
 - Highlighting and Note-Taking Neutron Data Of Structural Materials For
 - Interactive Elements Neutron Data Of Structural Materials For
8. Staying Engaged with Neutron Data Of Structural Materials For
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Neutron Data Of Structural Materials For
9. Balancing eBooks and Physical Books Neutron Data Of Structural Materials For
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Neutron Data Of Structural Materials For
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Neutron Data Of Structural Materials For
 - Setting Reading Goals Neutron Data Of Structural Materials For
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Neutron Data Of Structural Materials For
 - Fact-Checking eBook Content of Neutron Data Of Structural Materials For
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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