Estimation of uncertainties of displacement cross-sections for iron and tungsten at neutron irradiation energies above 0.1 MeV

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1. Introduction

The goal of the work is the evaluation of uncertainties of calculated atomic displacement cross-sections for iron and tungsten irradiated with neutrons. Uncertainties were analysed for neutron incident energies above 0.1 MeV making the main contribution to the value of radiation damage rate for different types of nuclear and fusion reactors, and neutron sources [1].

Covariance matrices for displacement cross-sections, σ_d were obtained using the Monte Carlo method described in Ref.[2]. The procedure consists of a) the choice of the "best" set of model parameters, b) the estimation of uncertainties of model parameters, c) the Monte Carlo sampling of N number of input data sets for the code used, iv) the execution of calculations for obtained N input data files, and v) the computation of covariance matrices for particular reactions

$$V_{ij} = N^{-1} \sum_{k=1}^{N} (\sigma_{d,ik} - \sigma_{d,i0})(\sigma_{d,jk} - \sigma_{d,j0}) \quad (1)$$

where $\sigma_{d,ik}$ is the displacement cross-section corresponding to the "i"-th primary neutron energy in the "k"-th Monte Carlo event, $\sigma_{d,i0}$ is the cross-section calculated using set of unchanged model parameters. The standard deviation of displacement cross-section is equal to

$$\Delta\sigma_{d,ii} = \sqrt{V_{ii}} \quad (2)$$

Recoil energy distributions were calculated for different input data sets using the TALYS-1.8 code [3] at incident neutron energies below 150 MeV and the CASCADE-2014 code [4,5] at energies above 100 MeV.

The uncertainties of displacement cross-section, σ_d were estimated using both the NRT model [6] and the arc-dpa approach [7,8].

When using the NRT model four parameters, α_i were varied. Three parameters α_1 - α_3 concern the numerical coefficients in g(e) formula [6] obtained in Ref.[9] by approximating the Lindhard's function:

$$g(\varepsilon) = 3.4008\,\varepsilon^{1/6} + 0.40244\,\varepsilon^{3/4} + \varepsilon\,, \quad (3)$$

The fourth parameter α_4 is the effective threshold displacement energy E_d.

Two parameters b_{arcdpa} and c_{arcdpa} [8] were varied when using the arc-dpa approach for iron and tungsten. In this case the parameters of the NRT formula applied [7,8] and E_d remained unchanged.

The variation of parameters of nuclear models and defect production models was done using a normal distribution. The Δp-value shown in figures and discussed below is the relative standard deviation (RSD) or the coefficient of variation concerning the σ/μ ratio of the distribution.

The criticism of the MC variation of NRT model parameters and the arguments for the variation are discussed in Refs.[10,11].

2. Incident neutron energies below 150 MeV

Energy and angular particle distributions, and recoil spectra were calculated using the TALYS-1.8 code. Optical model calculations were performed with the Koning-Delaroche potential [12].

The calculations for iron were made using TALYS with 6,700 MC-generated input data files, for tungsten with 3,200 input data files.

The recoil spectra for neutron elastic and inelastic discrete-level scattering (n,n') were obtained using calculated neutron angular distribution. A special procedure was applied to get recoil spectra for neutron inelastic continuum scattering using results of TALYS-1.8 calculations.

The contribution of shape elastic scattering in displacement cross-section calculated using the ECIS code [13] with a large number of MC-generated input data files is discussed in Ref.[10,11].

2.1 Iron

Fig.1 shows an example of the number of defects and defect production efficiency calculated with varied NRT and arc-dpa parameters with the RSD value equal to 20%. The effective threshold displacement energy E_d is equal 40 MeV.

Fig.2 shows the RSD values for the number of defects depending on different parameter variation.

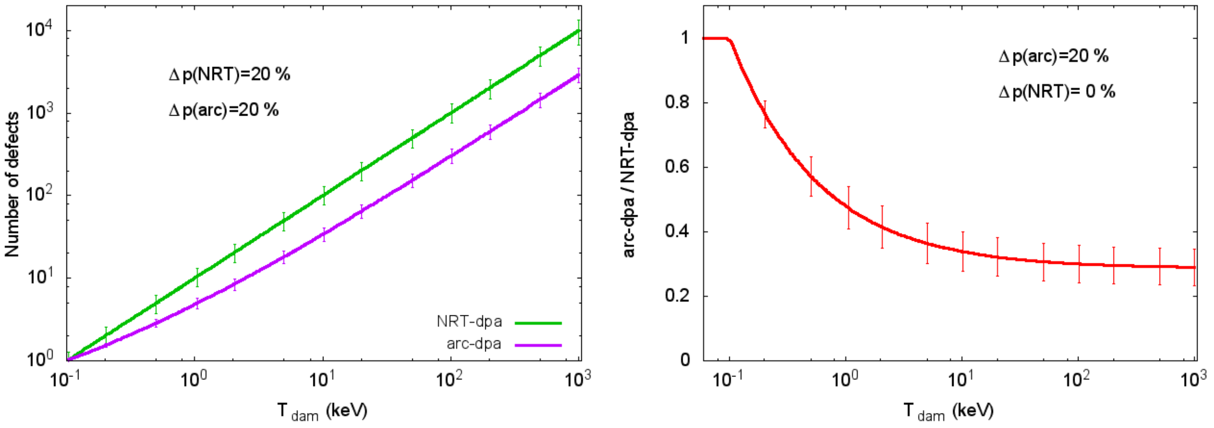

Fig.1 The number of defects calculated using the NRT model and the arc-dpa approach (left) and the efficiency of defect generation (right) calculated for iron with the coefficient of variation of NRT and arc-dpa parameters equal to 20%.

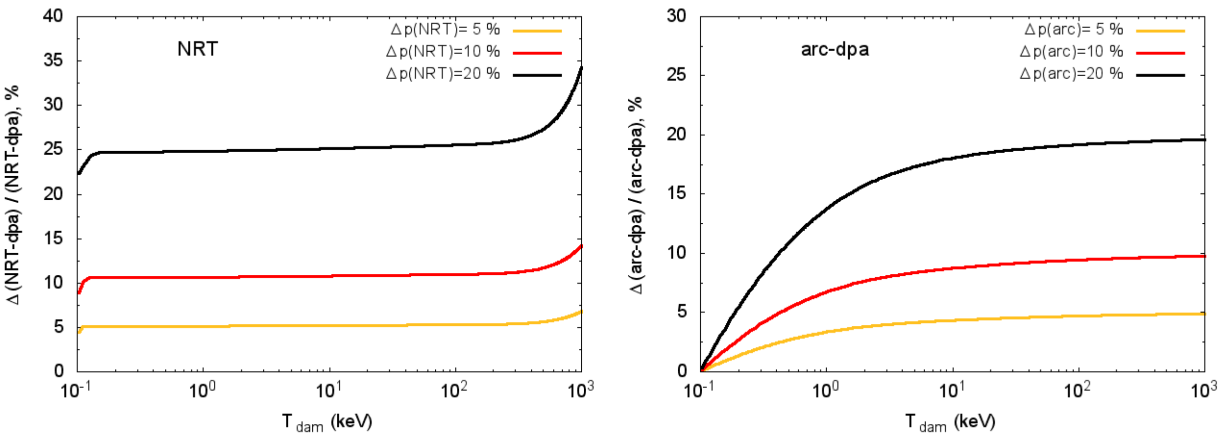

Fig.2 The RSD values for number of defects calculated using the NRT model and the arc-dpa approach for iron.

2.1.1 Components of displacement cross-section

Figure 3 and 4 shows examples of calculated RSD values for components of displacement cross-section obtained with the coefficient of variation of optical model parameters Δp(opt) equal to five percent and with the same coefficient for nuclear level density parameters Δp(levd) equal to ten percent. The resulting values $\Delta\sigma_{d,el}/\sigma_{d,el}$ are shown in Fig.3 for neuron elastic scattering and in Fig.4 for (n,2n) reaction.

The $\Delta\sigma_d/\sigma_d$ values for other reactions and results obtained with different variation of optical model parameters can be found in Refs.[10,11]. The influence of the adopted Δp(opt) value on the scatter of "common" cross-sections and the comparison with TENDL-2015 is also discussed in Refs.[10,11].

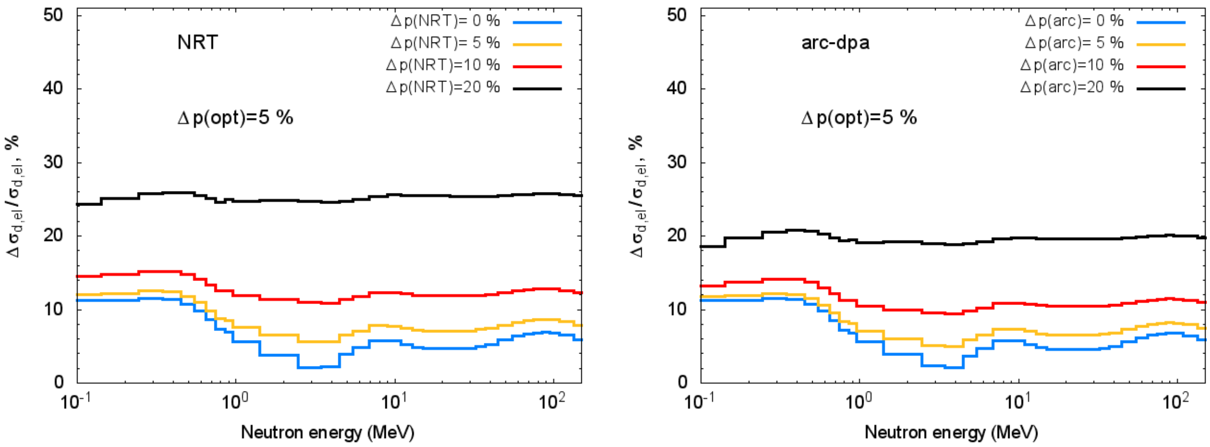

Fig.3 The RSD values for displacement cross-sections for neutron elastic scattering calculated using the NRT model and the arc-dpa approach for iron.

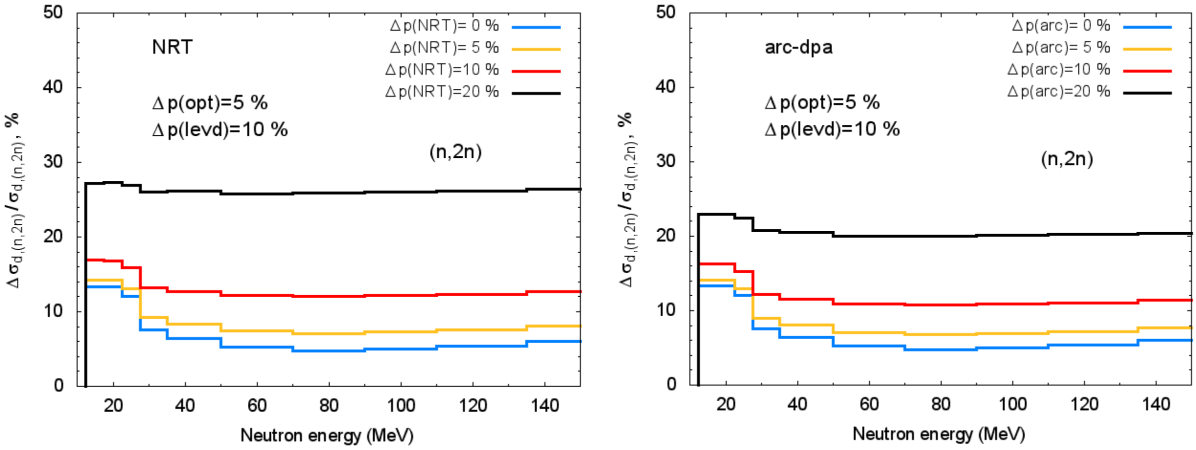

Fig.4 The RSD values for displacement cross-sections for the (n,2n) reaction for iron. See details in the text.

2.1.2 Total cross-section

Fig.5 shows RSD values for the total displacement cross-section calculated with different coefficients of variation of NRT, Δp(NRT) and arc-dpa, Δp(arc) parameters. The Δp(opt) and Δp(levd) values are equal to 5% and 10 % respectively. The results obtained with Δp(NRT) and Δp(arc) equal to zero illustrate the impact of the change of nuclear model parameters on the σ_d value.

The variation of NRT and arc-dpa parameters results to similar $\Delta\sigma_d/\sigma_d$ values.

The example of calculated displacement cross-sections with errors is shown in Fig.6. The additional information can be found in Refs.[10,11].

2.2 Tungsten

Fig.7 shows the $\Delta\sigma_d/\sigma_d$ values for total displacement cross-section calculated for tungsten. The Δp(opt) value is equal to 5 % and Δp(levd) is equal to 10 %. As in the case of iron the results of calculations using the NRT model and the arc-dpa approach are similar.

Fig.8 shows the example of calculated total displacement cross-sections with errors. The effective threshold displacement energy E_d for tungsten is taken equal to 70 MeV [8].

More information about $\Delta\sigma_d/\sigma_d$ for tungsten can be found in Refs.[10,11].

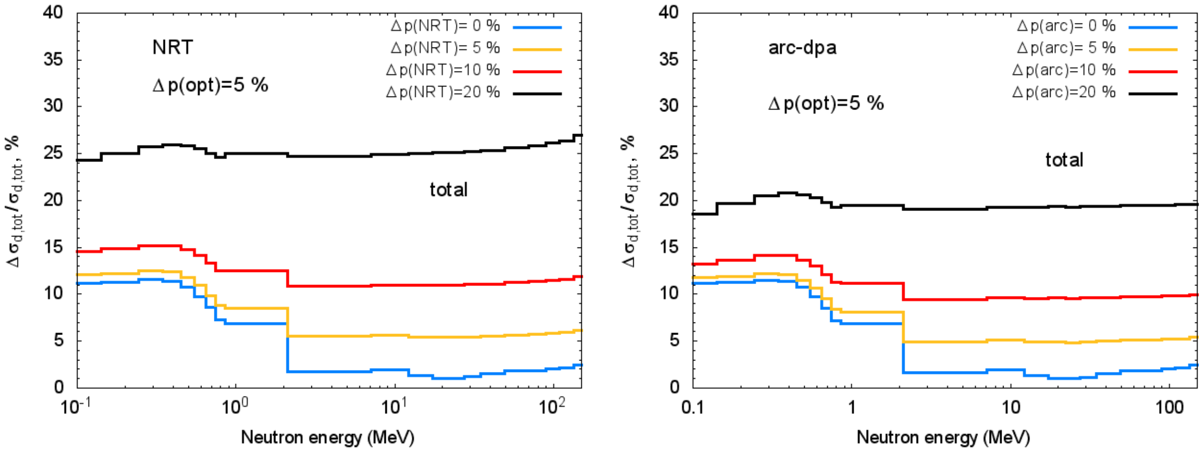

Fig.5 The RSD values for total displacement cross-sections for iron calculated using the NRT model and the arc-dpa approach.

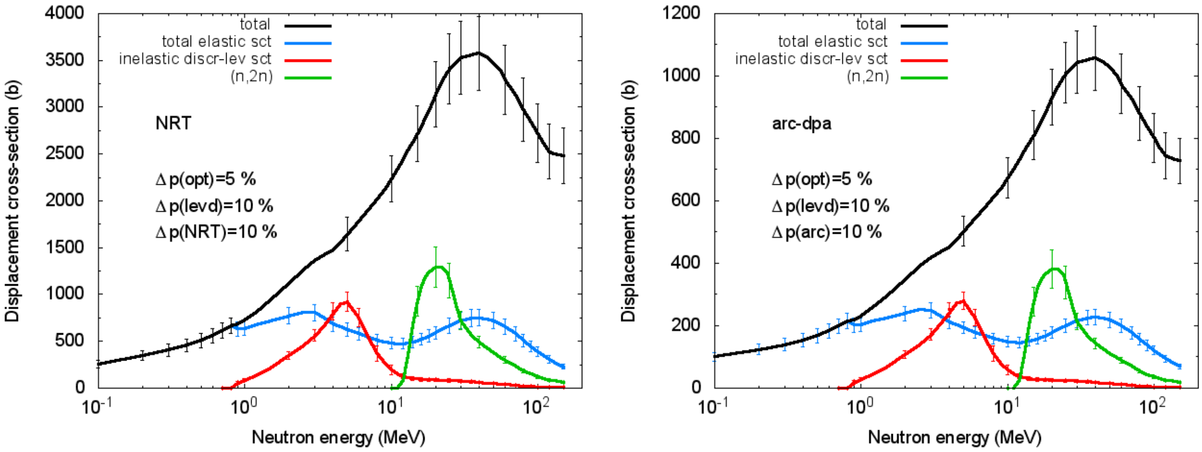

Fig.6 Example of total displacement cross-sections with errors calculated for iron using the NRT model and the arc-dpa approach. See explanations in the text.

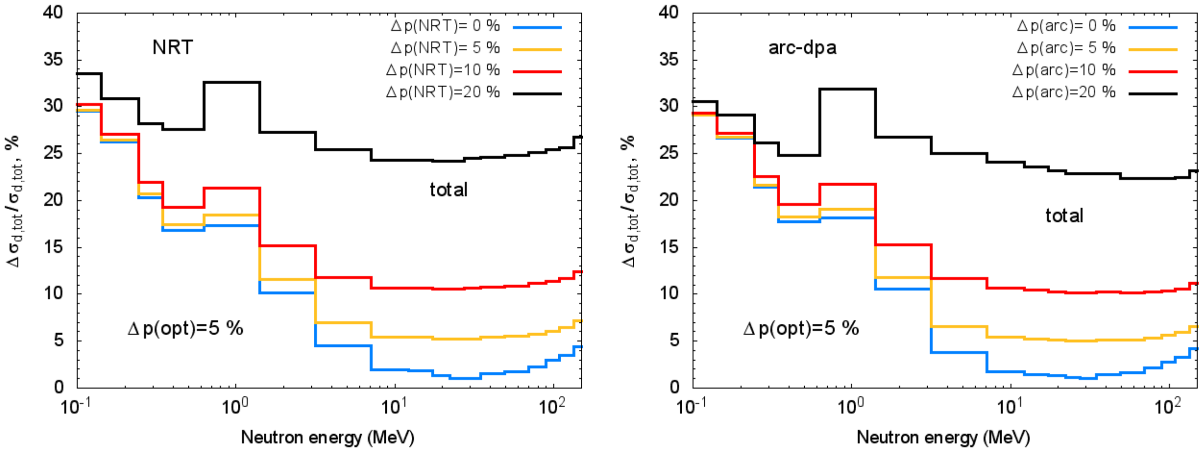

Fig.7 The RSD values for total displacement cross-sections for tungsten calculated using the NRT model and the arc-dpa approach.

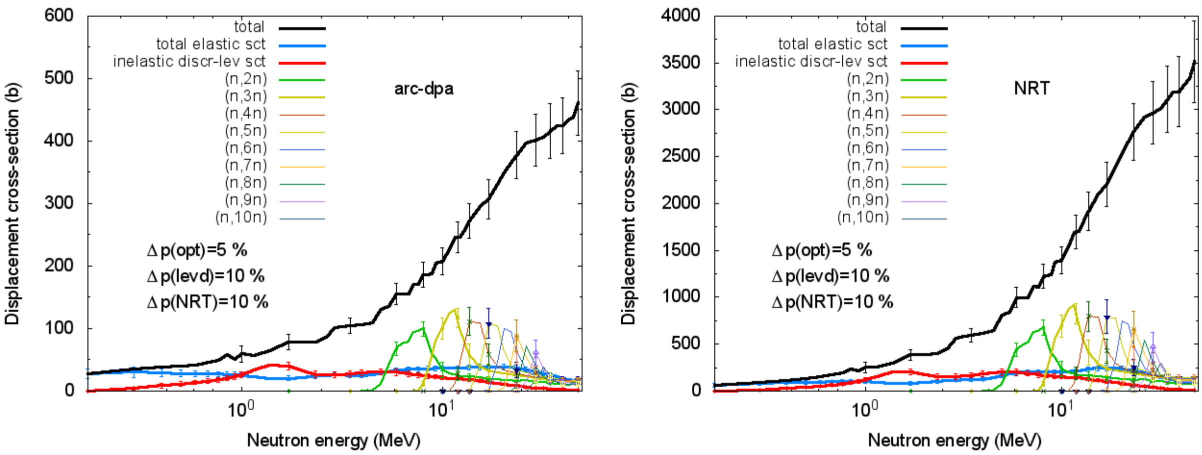

Fig.8 Example of total displacement cross-sections for iron calculated using NRT model and arc-dpa approach. The E_d value is equal to 70 eV.

3. Incident neutron energies up to 3 GeV

Fig.9 shows the example of RSD-value and displacement cross-sections calculated for neutron nonelastic interactions with iron using the CASCADE code. The following values concerning simulations with the intranuclear cascade evaporation model were varied, the corresponding RSD values are given in brackets: nuclear level density parameters (a: 10 %, δ: 20 %), nucleus radius (4 %), nucleon-nucleon and nucleon-pion cross-sections (10 %), total reaction cross-section used for the normalization of results (10%), and the NRT model parameters including E_d (from 0 to 20 %).

The results (Fig.9) seem to be close to values obtained using the TALYS code (Fig.5 left).

The scatter of displacement cross-sections calculated using different codes implementing intranuclear cascade evaporation model is discussed briefly in Refs.[10,11].

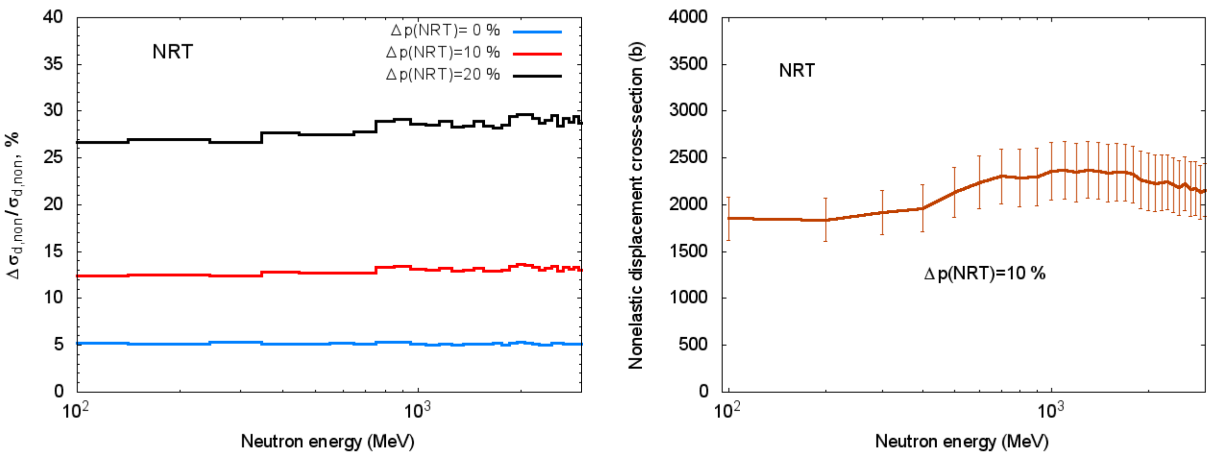

Fig.9 Example of $\Delta\sigma_d/\sigma_d$ values (left) and displacement cross-sections (right) for neutron nonelastic interactions with iron calculated using the CASCADE code at neutron incident energies from 100 MeV to 3 GeV. See details in the text.

4. Conclusion

Uncertainty of displacement cross-sections σ_d was evaluated for iron and tungsten irradiated with neutrons with energies from 0.1 MeV to 3 GeV. The TALYS [3] and ECIS [13] codes were applied for recoil energy distribution calculations in the energy range 0.1 to 150 MeV; the CASCADE code [4,5] implementing the intranuclear cascade evaporation model was used at the higher energies.

The NRT model [6] and the arc-dpa approach [7,8] were utilized to calculate the number of stable defects.

The RSD-values and correlation matrices for σ_d were obtained for different variation of optical model parameters, nuclear level density parameters, and parameters of models used for estimation of the number of defects produced under irradiation.

An additional study is needed to define the optimal range for possible variation of NRT and arc-dpa parameters.

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