Evaluation of Advanced Displacement Cross-Sections for the Major EUROFER Constituents Based on an Atomistic Modelling Approach

A.Yu.Konobeyev, U.Fischer, P.E.Pereslavtsev

Reliable assessments of radiation induced damage in fusion reactor materials require the use of advanced simulation techniques for the underlying displacement damage mechanisms. The calculation of radiation damage rates for the EUROFER reduced activation steel will be, therefore, based on improved displacement cross-sections based on molecular dynamics and binary collision approximation simulation methods for the calculation of the number of lattice defects. This approach shows a better agreement [1,2] with experimental data of point-defect production in materials that the standard NRT model [3] implemented in commonly used codes like the NJOY code [4].

In the present work the damage energy and displacement cross-sections data were evaluated for the main EUROFER constituents for neutron incident energies up to 150 MeV utilizing the advanced atomistic modelling approach combining the use of binary collision approximation model and results of molecular dynamics simulations. The data obtained were processed into ENDF and ACE formatted data and tested by means of MCNP calculations.

References

[1] A.Yu. Konobeyev, C.H.M. Broeders, U. Fischer, Improved displacement cross sections for structural materials irradiated with intermediate and high energy protons, Proc. 8th International Topical Meeting on the Nuclear Applications of Accelerator Technology (AccApp'07), July 30 - August 2, 2007, Pocatello, Idaho, USA, p.241.

[2] A.Yu. Konobeyev, U. Fischer, L. Zanini, Advanced evaluations of displacement and gas production cross sections for chromium, iron, and nickel up to 3 GeV incident particle energy, Tenth International Topical Meeting on Nuclear Applications of Accelerators (AccApp'11), Knoxville, TN April 3-7, 2011.

[3] M.J. Norgett, M.T. Robinson, I.M. Torrens, A proposed method of calculating displacement dose rates, *Nucl. Eng. Des.* 33 (1975) 50.

[4] NJOY: Data Processing System of Evaluated Nuclear Data Files in ENDF format, https://www.oecd-nea.org/dbprog/njoy-links.html