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TOPIC 4

FUELS AND MATERIALS

4.1 Radiation damage simulations & requirements

4.1.1 Introduction and current modelling capabilities

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Introduction

The selection of materials able to sustain intense radiation and severe environmental conditions is one of the major tasks for the design of any nuclear facility. Appropriate structural and functional materials for future fusion reactors are being developed now. Being on the cutting edge of technology this task presents a real challenge for material scientists and requires not only deep knowledge of material behavior under normal conditions, but also understanding of processes occurring in material under irradiation. This lecture is aimed at introduction of non-specialists into the basic physical phenomena taking place in irradiated metals.

Displacement damage in metals

After a short introduction into the major crystal lattice types elementary point defects in metals – vacancy and interstitial – and their properties will be discussed. Creation of point defects involves interaction of projectile with the atoms of target material. The details of such interaction depend mainly on the type of incident particles. Neutrons, gamma quanta or charge particles interact differently with matter. Therefore formally total displacement damage is subdivided in two parts: primary damage produced by incident particle and secondary one generated by the target atoms displaced from their lattice sites due to interaction with the projectile. Whether target atom will be displaced depends on the energy received from the projectile (energy transfer T) and the energy barrier necessary for irreversible defect creation (threshold displacement energy E_d). The last value is an important material parameter, necessary for displacement damage evaluation. Depending on the transferred energy several generations of recoil atoms can be created. In this way a cascade of atomic displacements can be formed in irradiated material.

As far as recoil atoms lose some fraction of their electrons and move in metals as charged particles it is necessary to consider in more detail ion interaction with irradiated material. The nuclear and electronic energy losses of charged ions in matter explain some features of cascade of atomic displacement development, which we demonstrate using TRIM calculations.

The Kinchin-Pease and NRT models for evaluation of the number of displaced atoms in cascades are discussed.

Time scales and stages of displacement cascade development will be considered on several examples of molecular dynamical simulations. The temperature in the cascade core can reach melting point stimulating defect diffusion, recombination and clustering. Defects in cascade are distributed very inhomogeneously: a vacancy reach core is surrounded by interstitial clusters at the periphery of cascade zone. Here we recall a qualitative model of in-cascade void formation proposed by R.S. Averback.

It should be noted that it is necessary to distinguish between

- the number of displacements in cascades calculated with, e.g., NRT, which corresponds to the peak disorder
- the number of defects survived after recombination phase, but still localized within the cascade area and

- the number of freely migrating defects, which corresponds to the average concentration of defects available for diffusion in the bulk (i.e. outside of the cascade zone).

Damage morphology depends on the projectile type and its energy. At high particle energies cascades are no more compact and break-up into subcascades. A model of subcascade formation proposed by M. Kiritani is discussed.
Evaluation of displacement damage is based on the notion of displacement damage cross section, which is discussed in general and in application to the case of neutron irradiation. Typical neutron damage cross sections, neutron spectra for various nuclear facilities and resulting primary knocked-on spectra are presented.
Finally several computer simulation methods of damage evolution are discussed with respect to their advantages and shortcomings.

Effects of irradiation on material properties
The effect of irradiation on materials is versatile. Several examples of the effect of irradiation on the increase of sample dimensions (swelling), the decrease of dynamical toughness (embrittlement) and mechanical properties degradation due to helium generated by nuclear transmutations are presented.

We show that, in spite of the widely spread opinion that irradiation induced swelling originate from excess of vacancies in the form of voids, volume increase is due to the interstitials which annihilate at free surfaces, grain boundaries and dislocations leaving excess of vacancies in the material bulk.

Mechanical test accessing material brittleness (Charpy impact test) and changes occurring under irradiation are explained by considering processes occurring at the microscopic level near crack tip. An example of reactor pressure vessel steel embrittlement due to the Cu-rich cluster precipitation is shortly discussed.

Transmutation induced helium increases material hardness, provokes formation of helium induced bubbles and may result in severe high temperature helium embrittlement. Some examples of these effects are presented.

Literature

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