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Understanding of neutron irradiation effect on zirconium alloys in nuclear systems

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1. Introduction

Nuclear reactor core materials are usually irradiated during the operation. Zirconium and zirconium alloys are normally used as fuel cladding materials in light water reactors. Because these materials have reasonable mechanical properties at normal operating condition and fairly low neutron capture cross section. To enhance the safety of cladding materials, especially zircaloy, under irradiation environment, it is necessary to understand microscopic changes of structures in materials in view of the safety enhancement and the life prediction of zirconium and its alloys. The aim of this study is to understand the fundamental behavior of zircaloy under irradiation.

2. Literature study of theoretical radiation effect

Irradiation effects on material begin with the kinetic energy of neutron and finish with lattice atom in materials. In order to understand the behavior of materials under irradiation, it is necessary to predict defects which exist and/or are produced in the materials.

2.1 Defect prediction

For the prediction of defect quantity, various data sets are needed, including fluence, neutron energy spectrum, atomic bonding force, lattice structure and cross-section. However, each data could be represented through three key parameters such as neutron flux, physical properties, and temperature. Flux and physical properties of material are involved in defect creation, and temperature is involved in defect annihilation. To understand neutron irradiation effect, it is useful to draw a perspective of atom behavior in terms of time scale as shown in Table. 1.

Table 1. Characteristic time scale [4].

Cascade creation	$\sim 10^{-13}$S
Unstable matrix	$\sim 10^{-11}$S
Interstitial diffusion	$\sim 10^{4}$S
Vacancy diffusion	~ 1S
Thermal diffusion	$\sim 10^{4}$S

Four sequences from the first, as shown in Table 1, determine defect quantity. The last sequence (thermal diffusion) mainly determines defect type and needs several orders of magnitude longer than 1sec.

Equations to predict defect quantity (damage equation and NRT model) are represented as below:

$$R_d = N \int_{\check{E}}^{\hat{E}} \Phi(E_i)\sigma_D(E_i)\mathrm{d}E_i \qquad (1)$$

Where *N = the lattice atom density,*
ϕ (Ei) = the energy-dependent particle flux
σ_D(Ei)= the energy-dependent displacement cross section.

$$\sigma_D(E_i) = \int_{\check{t}}^{\hat{t}} \sigma_D(E_i,T)\nu(T)\mathrm{d}T \qquad (2)$$

Where *σ_D(Ei,T) = the probability that a particle of energy Ei will impart a recoil energy T to a struck lattice atom*
ν (T) = the number of displaced atoms

$$N_d = \frac{k(E-S_e)}{2E_d} \qquad (3)$$

Where *E = the total energy of the PKA,*
S_e = the energy lost in the cascade by electron excitation
E_d = damage energy.

And thermal diffusion can be express by clustering rate equation:

$$\frac{dC_j}{dt} = \sum_k w(k;j)C_k - \sum_k w(j;k)C_j + G_j - L_j \qquad (4)$$

Where C_j= concentration of clusters of type j.
$w(j;k)$ = transition rate of cluster type k into j
G_j= form rate at which clusters of type j
L_j= loss rate of clusters of type j

To solve these equations, knowledge of many mechanisms is required including the detail analysis of diffusion behavior of each species. Also information of interaction parameters (threshold energy, crystallographic directions, atomic potential energy), and point defect generation are required.

3. Literature study of experimental results

Eventually defects will be interacted each other by thermal diffusion which will affect the determination of defect types. There are various types of defects including voids, dislocation lines, dislocation loops, vacancies, and interstitial atoms. Among these defects, dislocation is considered as one of the most important defects in zircaloy.

3.1 Zirconium main defect type: dislocation

<a> dislocation loops:

Point - defect clusters consist of perfect dislocation loops either of vacancy or interstitial nature with Burgers Vector 1/3 $<\mathbf{11\bar{2}0}>$ situated in the prismatic planes (at 250℃ and 400℃ and dose lower than 5 x 10^{25} nm^{-2}.

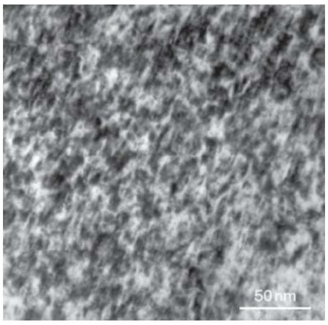

Fig.1. Typical <a> loop microstructure observed on recrystallized Zy-4 irradiated at 280℃ in Siloe´ up to a fluence of 6 x 10^{24} nm^{-2} [3].

<c> Component dislocation loops:

The <c> component loops have been analyzed as being faulted and of the vacancy type. They are located in the basal plane with a Burgers vector 1/6 $<\mathbf{20\bar{2}3}>$ having a component parallel to the <c> axis. The <c> component loops are much larger than the <a> loops but their density is much lower

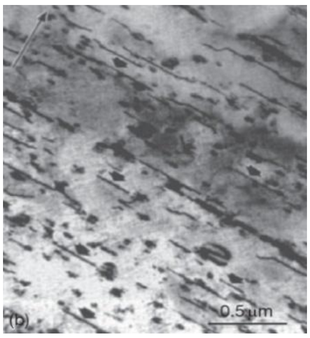

Fig.2. Sponge purity(2000 wt ppm) containing basal <c> component in an edge-on orientation (arrowed). Only <c> component defects are visible with diffracting vector of [0002]. The beam direction is $[10\bar{1}0]$ for each micrograph. [3].

4. Discussions

In order to unify the mechanism of neutron effect on zircaloy, the analysis of microstructures should be conducted in many scopes such as Kinetic theory (collision dynamics, reaction dynamic and recoil energy spectrum), atomic properties (point defect properties, point defect diffusion, point defect reaction). These scopes are extensive and wide, and it is hard to combine all information. And variables to determine microstructure changes are also many. It is not clear which variables give effects on the micro-structural change exactly.

5. Summary and conclusions

This study is focused on the understanding of radiation effects on microstructure of zirconium and its alloys. Both theory and experimental results represent defects in microstructure. The mechanism of neutron irradiation effect on zirconium and its alloys can be expressed by atomic reaction. Phase is considered that region of space, throughout which all physical properties of a material are essentially uniform. Therefore it is possible that each mechanism can be explained by phase. For instance, if irradiation condition is the same, microstructural change will be identical. Eventually phases can represent microstructure. So if process of this study goes on further, concept of phase can be combined by function which explains which variables give effects on the microstructure exactly. Concept of after irradiated phase can represent after radiation microstructure change.

6. References

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