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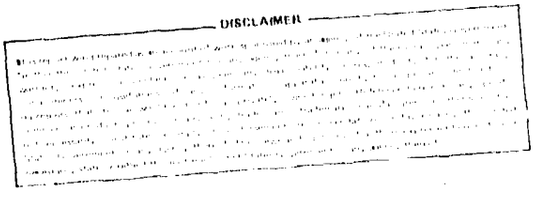

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DISPLACEMENT CASCADES IN POLYATOMIC MATERIALS*

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Using a continuous-slowing-down, random amorphous material model, we have studied displacement cascades in a number of diatomic materials. This paper reviews a number of previous results that elucidate the effects of atomic mass, recoil energy, displacement energy, capture energy and material stoichiometry on the numbers of displacements in a cascade. The displacement cascade reveals a complex structure that is dependent on the type of irradiation and the material properties. Conclusions related to damage analysis for fusion reactors are given.

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1. Introduction

The aspects of radiation damage analysis required for fusion reactor applications go beyond those encountered for fission reactors. In addition the range of neutron spectra, including 14 MeV neutrons, for which damage effects must be known, the class of materials that will be exposed to intense irradiation environments is much broader. Reactor concepts call for the use of structural alloys, structural and insulating ceramics, high temperature alloys, electrical conductors, organic insulators, and ordered alloys such as superconductors to be exposed to materials-limiting exposures. Although a great body of information is available on radiation effects in simple metals and important structural alloys, the picture of radiation effects in other materials in general is much less well understood.

When the basic problem of describing the displacement cascade in material such as ceramics and ordered alloys is considered, one finds that the theory developed for simple metals must be expanded. Factors that must now be considered include nonmetallic bonding, stoichiometry, new types of defects, mass effects, and multiple displacement thresholds.

In a series of papers we have investigated the nature of displacement cascades in polyatomic materials [1-4], including the special case of monatomic materials [5], using a continuous-slowing-down, random amorphous material model after the work of Lindhard et al. [6-8]. For most materials of interest, many relevant materials parameters, such as the displacement

thresholds, are not known; however, by doing a parametric study the important features of the displacement cascade can be elucidated.

In this paper we review a number of the important characteristics of the displacement cascade in polyatomic materials and discuss the implications for damage analysis of fusion reactors. The calculations presented are limited to the case of diatomic materials.

2. Equations for the net displacement function and the specified-projectile displacement function

Two functions that are useful in describing displacement cascades in polyatomic materials are the net displacement function, $g_{ij}(E)$, and the specified-projectile displacement function, $p_{ijk}(E)$. $g_{ij}(E)$ is the average number of type-j atoms displaced and not recaptured in subsequent replacement collisions in a displacement cascade initiated by a PKA of type i and energy E, and is analogous to the standard Kinchin-Pease result for monatomic materials. $p_{ijk}(E)$ is the average number of type-k atoms which are displaced from their sites by type-j atoms in a displacement cascade initiated by a PKA of type-i and energy E, and describes the specific collision events that produce displacements. Equations for $g_{ij}(E)$ and $p_{ijk}(E)$ are, respectively,

$$g_i(E) = \frac{dg_{ij}(E)}{dE} = \sum_k \sigma_{ik} \int_0^{M_{ik} E} dT \frac{d\sigma_{ik}(E,T)}{dT} \tag{1}$$

$$\times \left\{ p_k(T)\, g_{kj}(T - E_k^b) + [1 - p_k(T)\lambda_{ik}(E-T)] \right.$$

$$\left. \times g_{ij}(E-T) - g_{ij}(E) \right\} .$$

$$s_i(E)\,\frac{dp_{ijk}(E)}{dE} = \sum_{\ell} f_{\ell} \int_0^{M_{i\ell E}} \frac{d\sigma_{i\ell}(E,T)}{dT}\, dT$$

$$\times \Big\{ \rho_{\ell}(T)\left[\delta_{ij}\delta_{k} + p_{\ell jk}(T - E_{\ell}^{b})\right] \tag{2}$$

$$+ \left[1 - \rho_{\ell}(T)\lambda_{i\ell}(E - T)\right]\, p_{ijk}(E - T) - p_{ijk}(E) \Big\} .$$

The reader is referred to references [3] and [4] for a complete discussion of equations 1 and 2.

Beyond the values of Z and A for each element, the specific material properties are included via the atomic fraction f_{ℓ}, the displacement probability $\rho(T)$ and the trapping probability $\lambda_{i\ell}(E)$. In all calculations sharp-threshold approximations of ρ and $\lambda_{i\ell}$,

$$\rho_{\ell} = \begin{cases} 0, & T < E_{\ell}^{d} \\ 1, & T > E_{\ell}^{d} \end{cases}$$

$$\lambda_{i\ell} = \begin{cases} 1, & E < E_{i\ell}^{cap} \\ 0, & E > E_{i\ell}^{cap} \end{cases}$$

were used. Here E_{ℓ}^{d} is the average displacement threshold for type-ℓ atoms, and $E_{i\ell}^{cap}$ is the average capture energy below which a type-i atom will be trapped in a vacated type-ℓ site. In addition, it was always assumed that $E_{ii}^{cap} = E_{i}^{d}$ which corresponds to the Kinchin-Peace model for like atom collisions.

The effects of crystal structure, the nature of bonding, and the significance of type-i and type-j atom sites are approximated in the model calculations by appropriate choices of the parameters E_ℓ^d and E_{ij}^{cap}. In ionic crystals, for example, E_{ij}^{cap} for $i \neq j$ is most likely very small or zero. In ordered alloys a disordering replacement is a defect, whereas in a solution alloy it is not. Further, in these two cases it is probable that $E_{ij}^{cap} \simeq E_j^d$.

In discussing the results we have adopted the notation $A_xB_y(E_{11}^{cap}, E_{12}^{cap}, E_{21}^{cap}, E_{22}^{cap})$. This expression coupled with the assumption $E_{ii}^{cap} = E_i^d$ describes the parameters used in any calculation.

It is useful in investigating the properties of $g_{ij}(E)$ to define a set of displacement efficiencies k_{ij} by the relations

$$g_{ij} = \delta_{ij} + \bar{g}_{ij} = \delta_{ij} + k_{ij} f_j \nu_i / E_j^d \tag{3}$$

$$k_{ij} = \bar{g}_{ij} E_j^d / f_j \nu_i, \tag{4}$$

where ν_i is the damage energy for type-i atoms in the material [2].

The specific collision events that produce displacements are described by $p_{ijk}(E)$. The displacing atom fraction R_{ijk}, which is the fraction of the total number of type-k displacements that are produced by type-j atoms in a cascade initiated by a PKA of type i, is

$$R_{ijk} = p_{ijk} \left[\sum_\ell p_{i\ell}{}^k \right]^{-1}. \tag{5}$$

3. Discussion

3.1 Mass Ratio and Recoil Energy

Two important properties of k_{ij}, and hence g_{ij}, are shown by the results for MgO(62,00,00,62) in Fig. 1 and TaO(60,60,60,60) in Fig. 2. The results for MgO, a material with $M_1/M_2 \sim 1$, show that k_{ij} is a strong function of energy from threshold to the keV energy range and then is roughly constant for all higher energies, a result similar to that for monatomic materials [5]. Furthermore, the values of k_{ij} above a few keV are similar to each other, but with $k_{11} > k_{12}$. The TaO results demonstrate the behavior for a material with $M_1/M_2 \gg 1$. The same qualitative behavior is seen as or MgO, but with k_{ij} only becoming roughly constant after about 100 keV, and with $k_{11} \gg k_{12}$. The general observation is that in the threshold region, Region 1, k_{ij} is a strong function of energy; that is, $\bar{g}_{ij}$ is not proportional to damage energy. In the damage energy region, Region 2, k_{ij} is roughly constant, with $g_{ij} \approx \nu_i$.

These results show that the nature of the displacement cascade is a function of both material type and recoil energy. In materials whose mass ratio is near one (type-1 material) the number of displacements is approximately proportional to the damage energy for recoil energies resulting from fission and fusion neutron irradiation. This is not the case for Type-2 materials, ones whose mass ratio is far from one. Here the number of displacements is proportional to the damage energy only for 14 MeV neutron irradiations.

3.2 Stoichiometry

Two important factors in describing damage in polyatomic materials are the stoichiometry of the material and the stoichiometry of the displacement cascade. Our results show that the stoichiometry of the cascade is a function of materials property and recoil energy. To examine this behavior, let us consider the following ratio.

$$f_i = \frac{\bar{g}_{i1}}{\bar{g}_{i2}} = \left[\frac{k_{i1}}{k_{i2}}\right]\cdot\left[\frac{E_2^d}{E_1^d}\right]\cdot\left[\frac{f_1}{f_2}\right]. \qquad (6)$$

The term $[f_1/f_2]$ is just the concentration ratio for the material; and if the product of the terms in k_{ij} and E_j^d is one, then the cascade is stoichiometric. If the product is not equal to one, then there will be more net displacements on one sublattice than the other.

The values of the displacement thresholds in materials other than simple metals are not well known. Measurements in MgO have yielded results of 60 eV [9] and 69 eV [10] for both Mg and O and 57 eV has been measured for Zn and O in ZnO [11] . In Al_2O_3 a value of 18 eV for Al and 75 eV for O has been reported [12], and 40 and 20 eV thresholds have been reported for U and O, respectively, in UO_2 [13]. Although it is believed that the most physically reasonable situation is for very similar threshold values for the two atom types, the reported values for Al_2O_3 and UO_2 indicate the strong role E_j^d may play in determining cascade stoichiometry.

The final term to be considered is $[k_{i1}/k_{i2}]$. Selected values of $[k_{i1}/k_{i2}]$ at 10^7 eV are given in Table 1, which are representative of k_{ij} in Region-2. (Also see Figs. 1 and 2.) The results show that $[k_{i1}/k_{i2}] \neq 1$ in materials for which $M_1/M_2 \neq 1$. That is, the displacement cascade in polyatomic materials is not in general stoichiometric even for equal displacement thresholds. For the equal threshold case, in Type-1 materials like MgO or Al_2O_3, the deviation is 7-10%. For Type-2 materials like TaO, it is 60-80%.

Under conditions of unequal displacement thresholds in Type-1 materials the capture energy can effect the cascade stoichiometry. The Al_2O_3 calculations show a change of 45% between $E_{ij}^{cap} = 0$ and $E_{ij}^{cap} = 45$ eV. This does not occur in Type-2 materials, since capture does not occur or is unimportant for kinematic reasons [3].

The general conclusion is that the stoichiometry of the displacement cascade deviates from that of the host material, and that this deviation is a function of the threshold energies, mass ratio, capture energy, and recoil energy.

3.3 Specified-Projectile Displacement Function

The net displacement function g_{ij} describes the final condition of the cascade in our model, and its properties reflect the underlying displacement processes. These processes are poorly understood in polyatomic materials. The specified-projectile displacement function characterizes the displacement event by not only giving the displaced atom type but also the type of atom that displaces it.

The displacing atom fraction R_{ijk} calculated for the case MgO(62,62,62,62) is given in Figs. 3 and 4. For this Type-1 material the majority of displacing atoms are of the same type as the PKA. The results for TaO(60,60,60,60), a Type-2 material, are given in Figs. 5 and 6. The high-mass-atom sublattice plays the dominant role in producing displacements and, as can be seen in Fig. 6, at high energy it is even more important than the PKA sublattice. In all cases R_{ijk} becomes roughly constant only above 10^5 eV. The general conclusion is that the microscopic nature of the displacement processes in the cascade is dependent on the recoil energy and the material type. The recoil energy dependence shows that the displacement processes are changing over the entire range relevant to fusion neutron spectra.

4. Summary

The displacement cascade in polyatomic (diatomic) materials reveals a complex structure that depends upon the type of irradiation and the properties of the material. The net number of displacements was found to be proportional to the damage energy for recoil energies above a few keV for Type-1 materials and above $\sim 10^5$ eV for Type-2 materials. The stoichiometry of the displacements in the cascade differs from that of the irradiated material under all conditions studied. Finally, the specific collision events that produce displacements vary with recoil energy. These factors must be considered in evaluating radiation effects data in polyatomic materials for fusion reactor applications.

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Figure Captions

1) Values of the displacement efficiencies k_{ij} as functions of energy for the material MgO (62,00,00,62).

2) Values of the displacement efficiencies k_{ij} as functions of energy for the material TaO(60,60,60,60).

3) Values of R_{1ij} as functions of energy for the material MgO(62,62,62,62).

4) Values of R_{2ij} as functions of energy for the material MgO(62,62,62,62).

5) Values of R_{1ij} as functions of energy for the material TaO(60,60,60,60).

6) Values of R_{2ij} as functions of energy for the material TaO(60,60,60,60).

Table 1

Values of $[k_{i1}/k_{i2}]$ at 10^7 eV

	$[k_{11}/k_{12}]$	$[k_{21}/k_{22}]$
MgO		
(62,00,00,62)	1.08	1.09
(62,62,62,62)	1.07	1.09
Al_2O_3		
(18,00,00,72)	1.02	1.04
(18,45,45,72)	1.47	1.49
(60,60,60,60)	1.09	1.10
ZnO		
(60,00,00,60)	1.24	1.31
(60,60,60,60)	1.24	1.32
TaO		
(60,60,60,60)	1.61	1.80