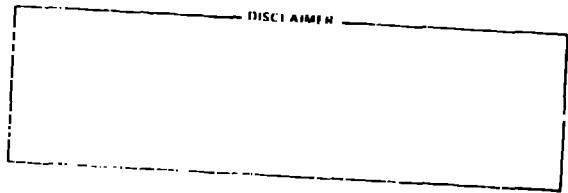LA-UR -81-2161

TITLE: DISPLACEMENT CASCADES IN DIATOMIC MATERIALS

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DISPLACEMENT CASCADES IN DIATOMIC MATERIALS*

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A new function, the specified-projectile displacement function $p_{ijk}(E)$, is introduced to describe displacement cascades in polyatomic materials. This function describes the specific collision events that produce displacements and hence adds new information not previously available. Calculations of $p_{ijk}(E)$ for MnO, Al_2O_3 and TaO are presented and discussed. Results show that the parameters that have the largest effect on displacement collision events are the PKA energy and the mass ratio of the atom types in the material. It is further shown that the microscopic nature of the displacement events changes over the entire recoil energy range relevant to fusion neutron spectra and that these changes are different in materials whose mass ratio is near one than in those where it is far from one.

1. INTRODUCTION

Polyatomic materials such as alloys, insulators and ceramics play an important role in many fusion reactor designs. The basic displacement process in these materials is more complicated and requires significantly more parameters for its description than is the case for monatomic materials. Consequently, the characteristics of displacement cascades produced in polyatomic materials by energetic particle irradiations are much less well understood than those produced in monatomic materials. In polyatomic materials the relative masses of the various atom types can have a strong influence on the numbers and types of defects produced, and new defect species can occur - e.g., those arising from disordering replacements. The description of displacement cascades in polyatomic materials thus requires the use of more complex functions than needed in the monoatomic case.

In previous studies we have investigated a number of the features of displacement cascades in polyatomic materials [1-3]. The approach used in these investigations was to calculate, as a function of the type and energy of the PKA producing the cascade, the damage energy deposited in the material; the total number of atoms of each species displaced; and the net number of these displaced atoms which were not subsequently recaptured in replacement collisions. These polyatomic damage energies and total and net displacement functions were evaluated for a number of diatomic materials and a few triatomic materials, and the results obtained provide much information about the general properties of displacement cascades in polyatomic materials. However, these three

functions still fail to determine a number of interesting intermediate and final features of a cascade's development.

We have therefore defined and studied two new functions characterizing displacement cascades in polyatomic materials, which contain all the information of the total and net displacement functions and much additional information which is missing from them. One of these new functions, which we term the specified-projectile displacement function, will be described here. It characterizes displacement events not only by the type of the atom displaced but also by the type of the atom that displaces it - which, of course, is frequently not the same as the type of the PKA which initiated the cascade. The second function, which characterizes the precise nature of all replacement events, will be discussed in a future paper.

2. The Specified-Projectile Displacement Function

The specified-projectile displacement function $p_{ijk}(E)$ is defined as 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. The PKA itself is not counted by $p_{ijk}(E)$. An integrodifferential equation to determine the specified-projectile displacement function can be derived by the methods of Linhard et al. [4-6] and our previous studies [1-3]. Let

$$\frac{d\sigma_{ij}(E,T)}{dT}$$

be the differential scattering cross section for a moving type-i atom with energy E to elastically transfer kinetic energy T to a type-j atom, $p_j(T)$ the probability that the type-j atom will then be displaced, E_j^b the binding energy (it

loses in the displacement process, and λ_{ij} (E-T) the probability that the incident atom (left with energy E-T after the collision) will be trapped in the vacated type-j site. In addition, let $M_{ij} \equiv 4M_iM_j/(M_i + M_j)^2$ be the kinematic energy transfer efficiency for the collision, $s_i(E)$ the electronic stopping power of the material per unit atom density for a type-i atom of energy E, and f_i the atomic fraction of type-i atoms in the material. The equation for the specified projectile displacement function is then

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

$$\times \{\rho_\ell(T) [\delta_{ij}\delta_{k\ell} + p_{\ell j k}(T - E_\ell^b)] \quad (1)$$

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

where the sum over ℓ is over all atom types in the material. In the first bracket term in the integral, $\rho_\ell(T)$ gives the probability that a displacement occurs; and the first term in the bracket counts the resulting contribution to p_{ijk} if the incident and struck atoms are of the proper types, while the second term in the bracket counts subsequent effects of the displaced atom. The second bracket term takes account of subsequent effects of the incident particle itself provided it is not captured in the current collision (probability $[1 - \rho_\ell(T)\lambda_{i\ell}(E-T)]$). Finally, the last term in the integral and the term on the left of the equation arise from motion of the atom of type i with electronic energy loss, but with no atomic collision [2].

For all the calculations discussed here, sharp-threshold forms of ρ_ℓ and $\lambda_{i\ell}$ were assumed; i.e.,

$$\rho_\ell = \begin{cases} 0, & T < E_\ell^d \\ 1, & T > E_\ell^d \end{cases} \quad (2)$$

$$\lambda_{i\ell} = \begin{cases} 1, & E < E_{i\ell}^{cap} \\ 0, & E > E_{i\ell}^{cap} \end{cases} \quad (3)$$

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. It was also assumed in the calculations that $E_\ell^b = 0$ and $E_i^{cap} = E_i^d$ (cf. [3]). In describing our results for diatomic materials below we have used the notation $A_xB_y(E_{11}^{cap}, E_{12}^{cap}, E_{21}^{cap}, E_{22}^{cap})$, with the

E_{ij}^{cap} expressed in eV, to characterize the material. In conjunction with the above assumptions, this format provides a complete description of the material parameters used in a calculation. The values of the p_{ijk} are actually quite insensitive to the choice of the E_{ij}^{cap} for $i \neq j$; thus even though particular choices of these latter parameters were made in the calculations discussed in the next section, the results can be considered to be essentially independent of those choices.

3. RESULTS

Once a set of material parameters is chosen, Eq. (1) may be numerically integrated to determine the $p_{ijk}(E)$. Note that $p_{ijk}(E)$ is not the total number of type-k atoms displaced in the cascade initiated by the PKA of type i and energy E, but only the subset of them which are displaced upon being struck by type-j atoms - hence the name "specified-projectile" displacement function. A determination of how the number of displacements per cascade for a given projectile atom type j and displaced atom type k depends on the properties of the material is clearly needed for an understanding of displacement cascades in polyatomic materials.

Using certain choices of the E_{ij}^{cap}, we have calculated the specified-projectile displacement functions for the diatomic materials MgO, Al$_2$O$_3$, and TaO. It is convenient to describe the results obtained by introducing the displacing atom fraction $R_{ijk}(E)$, defined as

$$R_{ijk}(E) \equiv p_{ijk}(E)/\sum_\ell p_{i\ell k}(E). \quad (4)$$

For a cascade initiated by a PKA of type i and energy E, $R_{ijk}(E)$ is that fraction of the total number of type-k displacements that was produced by type-j atoms.

First consider the case MgO(62,62,62,62), where the two atomic species occur in equal numbers and have relatively similar masses, and where all the displacement thresholds and capture energies are the same. Values of the $R_{ijk}(E)$ for this situation are shown in Figs. 1 and 2. Note that the asymptotic values of the
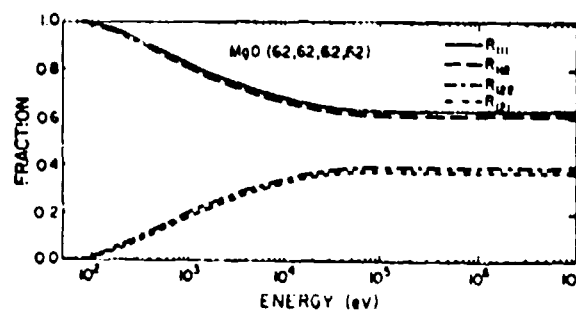
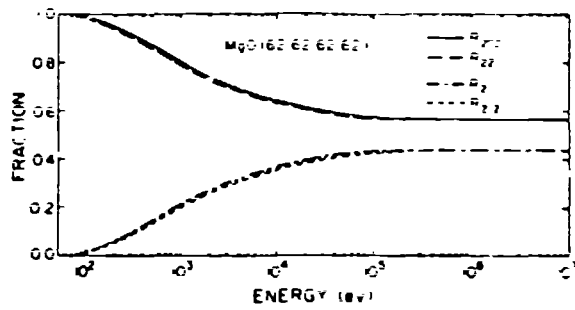Figure 1. Values of the ratio R_{ijk} for the material MgO (62,62,62,62) as a function of PKA energy.

Figure 2. Values of the ratio R_{21k} for the material MgO (62,62,62,62) as a function of PKA energy.
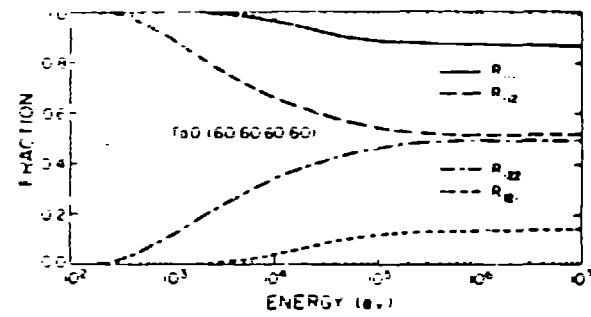

Figure 3. Values of the ratio R_{11k} for the material Al_2O_3 (18,45,45,72) as a function of PKA energy.

Figure 4. Values of the ratio R_{21k} for the material Al_2O_3 (18,45,45,72) as a function of PKA energy.

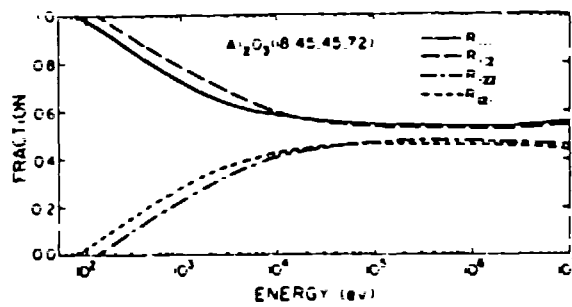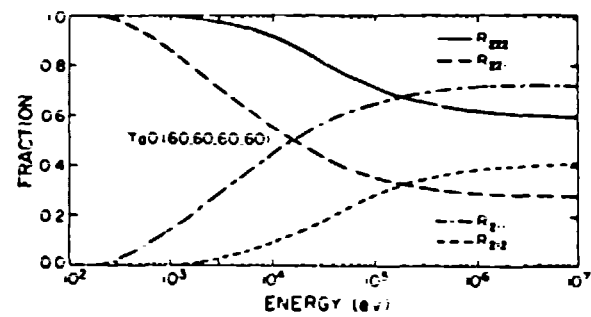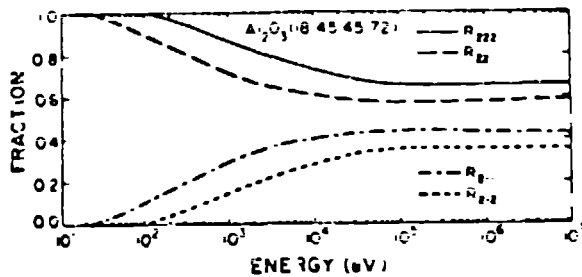Figure 5. Values of the ratio R_{11k} for the material TaO (60,60,60,60) as a function of PKA energy.

Fig 6. Values of the ratio R_{21k} for the material TaO (60,60,60,60) as a function of PKA energy.

R_{iik} are not equal to 0.5, and that they are not the same for Mg as for O PKA's. In addition, all the R_{iik} are greater than any of the R_{ijk} with $i \neq j$ due to the generally greater efficiency of energy transfer between equal-mass atoms (cf. [2]). Finally, Mg atoms in Mg-initiated cascades are more effective in producing displacements than are O atoms in O-initiated cascades, primarily because the heavier atoms dissipate less kinetic energy through electronic excitation [2].

Figs. 3 and 4 show results obtained for the case Al_2O_3(18,45,45,72), with the choice of displacement thresholds based on the work of Pells and Phillips [8]. The masses of the two atom types are again relatively similar, but now the two species appear with different atomic fractions and have quite different displacement thresholds. $R_{121}(E)$ is larger for Al_2O_3 than for MgO primarily because at energies near the threshold for an Al atom to displace an O atom, where R_{121} becomes nonzero, the low threshold for Al makes it more probable for an O atom to displace an Al atom than another O atom. A similar effect is seen for $R_{211}(E)$. As the PKA energy increases this unequal-threshold effect becomes less important. The stoichiometric effect of the relatively greater number of O atoms in the material displays itself in the fact that, away from threshold, the R_{12k} are all greater than in the case of MgO.

Results for the material TaO(60,60,60,60) are shown in Figs. 5 and 6. In this case the atomic fractions, displacement thresholds, and capture energies are all the same, but the Ta mass is much greater than the O mass. The dominant role of the high-mass atom in the displacement process is evident in the figures; one sees that $R_{111} \gg R_{121}$ at all energies, and at high energies $R_{112} \lesssim R_{122}$. Also note that the

displacement of an atom by another atom of the same kind occurs more frequently than in the case of MgO, where the two atomic masses are more nearly equal. A particularly striking example of the heavy-atom dominance can be seen in displacement cascades with O PKA's; above 10^3 eV the value of R_{211} becomes considerably greater than that of R_{221}, showing the enhanced efficiency of getting energy into moving Ta atoms.

It is seen that for all the cases considered the asymptotic values of $R_{ijk}(E)$ are not reached until $E \gtrsim 10^5$ eV. Thus until rather large PKA energies are reached the specific collision events which produce displacements are changing. The general energy dependence of $R_{ijk}(E)$ is somewhat similar to that observed for the distribution of displaced atom types [3].

4. Conclusion

The specified-projectile displacement function $p_{ijk}(E)$ describes the specific collision events that produce displacements. By calculating values of this function for several types of diatomic materials, we have found that the two parameters that have the largest effect on the displacement collision events are the PKA energy and the mass ratio of the atom types in the material. It is of consequence to studies of polyatomic materials for fusion reactor applications that the microscopic nature of the displacement events is changing over the entire recoil energy range relevant to fusion neutron spectra, and that these changes are quite different in materials where the mass ratio is near one than in those where it is far from one.

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