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LETTER TO THE EDITORS

DISPLACEMENT ENERGIES FOR Zr MEASURED IN A HVEM

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1. Introduction

A critical factor in determining the displacement cross-section (σ) for incident particles of a given energy is the effective threshold displacement energy (T_e), i.e. the energy of an incident particle (T) above which the probability of displacement (P_d) is 1 for a randomly directed knock-on when the energy transferred is a maximum. Expressions for σ vary according to the energy, mass and charge of the incident particle [1]. Tabulated values of σ for incident particles of various energies are available for electrons [2] and neutrons [3]. The number of displacements per atom (dpa) experienced by a crystal as a function of fluence (ϕt) for a given neutron spectrum can then be determined according to:

$$\text{dpa} = \sigma\phi t.$$

Various values of T_e for Zr have been reported in the literature. Neely [4] estimated a value of 28 eV based on resistivity measurements after electron irradiation at 8 K. The minimum threshold energy (T_d) was measured at 24 eV but the effective value of 28 eV was quoted as the best value to fit a single step displacement energy curve for polycrystalline Zr and, as such is presumably an average value over all orientations. For most practical applications a single-step displacement energy curve such as this is used for dpa calculations. Displacement rates are generally required for polycrystalline material subject to multiple displacement events, for example during neutron irradiation, and therefore an estimated average value of T_d over all orientations is normally used.

Biget, Maury, Vajda, Lucasson and Lucasson [5] proposed a complex step function for P_d as a function of T (the energy of the incident particle) to fit their experimental data (for electron irradiation of Zr at < 8 K) which more accurately reflected the marked anisotropy of the hexagonal lattice:

$P_d = 0$ for $T < 21$ eV,
$= 0.16$ for $21 < T < 30$ eV,
$= 0.55$ for $30 < T < 50$ eV,
$= 0.61$ for $50 < T < 110$ eV.

The minimum threshold energy was estimated at 21 eV. They suggested that each step of the displacement probability curve corresponded to the displacement energy of low index easy displacement directions. In a review of threshold displacement energies, Kenik and Mitchell [6] fitted an orientation dependence to the values given by Biget et al. [5] that was similar to that for other close-packed metals such as Zn [7]. Their values are shown in table 1.

This paper describes direct measurements of threshold displacement energies for Zr obtained by electron irradiation in a high voltage microscope (HVEM) and compares the measurements with the earlier data.

2. Experimental

Threshold displacement energies for Zr ($> 99.95\%$ pure) were measured using an AIE EM7 high voltage electron microscope (HVEM) at Birmingham University

Table 1
Threshold displacement energies (T_d) as a function of orientation for Zr derived from resistivity data [5]

	Orientation				Reference
	[0001]	$\langle 11\bar{2}3\rangle$	$\langle 10\bar{1}0\rangle$	$\langle 11\bar{2}0\rangle$	
T_d (eV)	50.0	–	30.0	21.0	[9]

Table 2
Threshold displacement energies (T_d) as a function of orientation for Zr determined from the production of visible damage in a HVEM at about 300 K

	Orientation				Reference
	[0001]	$\langle 11\bar{2}3\rangle$	$\langle 10\bar{1}0\rangle$	$\langle 11\bar{2}0\rangle$	
T_d (eV)	25.5 ± 0.5	24.0 ± 0.5	24.5 ± 1.0	27.5 ± 1.0	[8]

and at the Max Planck Institut in Stuttgart. Electron transparent thin foils were irradiated at room temperature for a range of accelerating voltages up to 1 MeV. The threshold energies were determined from the electron energies required to produce visible damage in the form of small (about 5 nm diameter) dislocation loops.

3. Results and discussion

Direct measurements of threshold displacement energies obtained using the HVEM at Birmingham University are listed in table 2 for each of four low index zone axes. They show that the average value of T_d is about 25 eV and that T_d $[11\bar{2}0] > [0001] > [10\bar{1}0] > [11\bar{2}3]$. In some cases the damage first appeared close to the surface of the foils indicating that the displacement energies were influenced by surface effects. This is possible if threshold energies are lowered by knock-on effects from oxygen in the surface oxide or by increases in the lattice parameters close to the surfaces due to oxygen dissolution [8]. Care was taken to ensure that damage was produced within the bulk of the foils for a valid threshold energy. There may be some error in the measurements because of surface effects, however, the orientation dependence for T_d is unlikely to be significantly affected. The measurements obtained on the Birmingham HVEM are consistent with measurements recently obtained on the HVEM at Stuttgart showing T_d $[11\bar{2}0] < 34$ eV (800 kV) and T_d $[0001] < 24$ eV (700 kV).

The orientation relationship for threshold energies described above is not consistent with that derived by Kenik and Mitchell [6] from the data of Biget et al. [5]. The reason for the discrepancy can be attributed to the fact that Kenik and Mitchell presumably assigned an orientation relationship to Biget et al.'s data for Zr assuming that it was the same as that measured for other hexagonal close-packed metals such as Zn and Cd, i.e. T_d $[0001] > [10\bar{1}0] > [11\bar{2}0]$. The HVEM measurements show that this is not a valid assumption for Zr and the orientation relationship is effectively reversed with T_d $[11\bar{2}0] > [0001]$. This reversal can be understood if one considers that Zn has a c/a ratio (1.856) which is higher than the ideal packing ratio (1.633) and Zr has a c/a ratio (1.593) which is lower than the ideal packing ratio. The shortest bond distances are $\frac{1}{3}\langle 11\bar{2}0\rangle$ for Zn, $\frac{1}{6}\langle 20\bar{2}3\rangle$ for Zr and the largest interplanar spacings are (0002) for Zn, $(10\bar{1}0)$ for Zr. One can conclude that these factors determine whether the minimum threshold energy is along $[11\bar{2}0]$, as in the case of Zn, or [0001], in the case of Zr. This argument is supported by the fact that an orientation dependence similar to that of Zr has been measured for Ti [9] which, like Zr, has a c/a ratio (1.587) less than the ideal value for close-packed spheres.

It could be argued that threshold displacement energies measured in a HVEM are not comparable with resistivity measurements because of the differences in the two methods. Firstly, the threshold displacement energies obtained in an electron microscope may be regarded as upper limits because of the requirement for the production of visible damage clusters. Secondly, the data are obtained at different temperatures and it has been shown by Urban [10] that T_d can be strongly temperature dependent, decreasing with increasing temperature. This is consistent with the results of Karim et al. [7] indicating a general disagreement between resistivity data (obtained at about 8 K) and HVEM data (obtained at about 300 K). There is a tendency for lower values in the latter case. Even though it is difficult to compare HVEM with bulk resistivity data for the determination of threshold energies, it can be argued that threshold measurements obtained at low temperatures (about 8 K), by the resistivity method, may not be valid for applications at nuclear reactor operating temperatures. Therefore, measurements obtained in the HVEM (at temperatures > 300 K) may be considered to be more applicable for practical applications.

4. Conclusions

The threshold displacement energy for the production of visible damage in Zr irradiated with electrons in a HVEM is dependent on the crystallographic orientation with respect to the beam of bombarding particles. The average value for the four crystallographic directions listed in table 2 is about 25 eV for irradiation at about 300 K. The orientation dependence of the threshold displacement energies for Zr, which has a c/a ratio less than the ideal value (1.633), is different from other hexagonal materials having c/a ratios greater than the ideal value.

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