***Ab Initio* Prediction of Threshold Displacement Energies in ZrC**

Ming-Jie Zheng^{a,b,c}, Izabela Szlufarska^{a,d}, Dane Morgan^{a, d, *}

^a*Department of Materials Science and Engineering, University of Wisconsin- Madison,
Madison, Wisconsin, U.S.A.*

^b*Institute of Nuclear Energy Safety Technology, Chinese Academy of Sciences, China*

^c*Key Laboratory of Neutronics and Radiation Safety, Chinese Academy of Sciences,
China*

^d*Materials Science Program, University of Wisconsin- Madison, Madison, Wisconsin,
U.S.A.*

* Corresponding author's email: ddmorgan@wisc.edu

Abstract

The threshold displacement energies (E_d) of C and Zr atoms in ZrC have been determined using *ab initio* molecular dynamics simulation. The values of E_d have been predicted along the three main high-symmetry crystallographic directions [001], [011], and [111], and the averaged E_d values are 16 eV and 37 eV for the C and Si sublattices, respectively.

We further explore the dependence of E_d on small deviations from these high-symmetry directions and on the presence of C vacancies, which are often encountered in ZrC_x alloys. The trends in values are explained in terms of the structural and chemical properties of ZrC. The predicted E_d values provide relevant parameters for future modeling of radiation damage in ZrC.

1. Introduction

Zirconium carbide (ZrC), due to its high temperature stability, oxygen gettering ability, chemical inertness and resistance to irradiation damage[1-3], is of interest as a radiation resistant structural material in the high temperature gas cooled reactor (HTGCR). However, the radiation responses of ZrC are still poorly understood, including both its high-temperature microstructural changes [4] and the origin of its superior resistance to amorphization. In fact, radiation-induced amorphization of ZrC has not yet been observed experimentally at any temperature or dose [1, 4-10]. One of the key unknown parameters needed to model the irradiation response of ZrC, e.g., using SRIM simulations[11], is the threshold displacement energy (E_d).

E_d has several different definitions [12-15] and in this work we follow Ref. [15] and it is defined as the minimum kinetic energy required to produce a permanent defect on the same sublattice as the PKA, such as a stable Frenkel pair, which may or may not involve displacement of the PKA. Please see the Appendix for results following a

somewhat different definition. The Kinchin-Pease and Norgett-Robinson-Torrens (NRT) models for Frenkel pair defect production under irradiation predict that Frenkel pairs will be produced by a high-energy ion in a quantity inversely proportional to the value of E_d [16]. The widely used SRIM code [11] for predicting defect production rates also requires E_d values as input. In addition, in some cases the E_d values have been associated with a material's amorphization resistance[17]. For example, in a molecular dynamics (MD) simulation of ion beam irradiation on GaN[18], the high E_d values were used to help explain the small initial damage and high dose to amorphization of GaN. It is possible that E_d values in ZrC (if they are sufficiently high) could be responsible for the unusual resistance of this material to amorphization. It is also of fundamental interest to explore if the unusual structural aspects of ZrC, in which C behaves almost like an interstitial and which can tolerate a very large number of C vacancies (a large x in ZrC_x), produces unusual values of E_d compared to nominally similar materials, e.g., SiC. In general E_d is not isotropic, which means that it can have different values for different crystallographic directions and for symmetry distinct atoms.

The value of E_d is difficult to measure experimentally, since a single defect is hard to create in irradiation experiments, and even if it can be generated, it is difficult to identify [12]. Among the computational methods, the molecular dynamics (MD) technique has been proved to be an effective and efficient way to predict threshold displacement energies [12, 19-20]. MD simulations can be performed using classical

interatomic potentials (which we will call Classical MD (CMD)) or *ab initio* calculations (which we will call *Ab Initio* MD (AIMD)). Although AIMD is far slower and more computationally demanding than CMD, it avoids the use of interatomic potentials, which have been suggested to be the largest source of errors in E_d values determined with CMD [21]. AIMD has previously been successfully applied to study E_d in SiC [12], GaN [20], and $\text{Y}_2\text{Ti}_2\text{O}_7$ [22].

Threshold displacement energies in ZrC have been previously estimated by Gosset et al. [5] who found E_d to be equal to 25 eV and 35 eV for C and Zr, respectively. However, these values were estimated based on experimentally observed values in TaC rather than in ZrC. E_d for ZrC has not been measured or calculated directly. Furthermore, no information about the anisotropy of E_d or the possible influence of ZrC_x ($x < 1$) off-stoichiometry on E_d is known.

In this work, we use AIMD simulation to calculate the E_d in ZrC. To explore anisotropy, we predict E_d along different directions for the primary knock-on atom (PKA), considering displacements both directly along high-symmetry and slightly off high-symmetry directions. We also investigate effects of the off-stoichiometric properties of ZrC_x ($0.6 < x < 0.98$)[2] by predicting the influence of C vacancies on E_d .

2. Methods

The AIMD simulations were performed with the Vienna Ab-initio Simulation Package (VASP)[23-26] in the framework of density functional theory (DFT) and the projector-augmented wave (PAW) method. The exchange-correlation was treated in the generalized gradient approximation (GGA), as parameterized by Perdew, Burke, and Ernzerhof (PBE)[27]. The PAW potentials were generated with the following valence electronic configurations: $5s4d5p$ for Zr and $2s^22p^2$ for C. An energy cut-off of 450 eV was used.

We used a $3\times3\times3$ cubic supercell of ZrC containing 216 atoms. The system-size convergence was verified by comparing the corresponding E_d values in a 64-atom cell with those in a 216-atom cell, as shown in Table A.1 in the Appendix. It was found that the values agree within 5 eV except for Zr[001], where the 64 atom cell gives a large error due to a periodic boundary effect. This agreement suggests that the results for the 216-atom cell are well converged with respect to size to within a few eV or less. The large discrepancy for $E_d(\text{Zr}[001])$ in these two supercells is due to a "wrapping" error in the 64-atom cell, where the collision wraps across the periodic cell and the energy from the PKA effectively interacts with itself, causing a large reduction of E_d . No such obvious "wrapping" effects occurred for the 216-atom supercell simulations. In all AIMD runs, we use a single gamma point for the k-points.

Three steps are used for the AIMD simulations. In the first step, the system is equilibrated at 300K using a Nose-Hoover thermostat (the equilibration runs). The time

step is 1fs and the equilibration time lasts 1ps. In the second step, a series of initial kinetic energies are added to the PKA to attempt to generate Frenkel pairs (the production runs). No thermostat is used in this step. The time step is 0.1fs, which was found to give a maximum displacement during one AIMD time step of about 0.02 Å, as measured in simulations for C PKA with an initial kinetic energy of 50 eV. We believe this time step is small enough as this associated maximum displacement is lower than the maximum displacement of 0.1 Å recommended by Corrales et al.[28] for calculations of excess energy in displacement cascades. After simulating for about 0.2ps, we are able to observe whether a Frenkel pair will form or not at the given kinetic energy and thereby roughly estimate the value of E_d . To determine E_d , a velocity corresponding to the kinetic energy (E_k) was given to a C (or Zr) PKA atom. The PKA velocity was initially aligned along the three main crystallographic directions: [001], [011], and [111], as shown in Figs. 1 (a) and (b). We have also checked the effects of tilting the velocity direction slightly off the high-symmetry directions (by a small angle of about $\alpha \approx 2^\circ$). To define the tilted directions, we use the unit vector triplet ($\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$) to describe the velocity directions. As we know, the unit vectors along the [001], [011], and [111] are (0, 0, 1), (0, $\sin 45^\circ$, $\cos 45^\circ$), and ($\sin 55^\circ \cos 45^\circ$, $\sin 55^\circ \sin 45^\circ$, $\cos 55^\circ$), respectively. The corresponding unit vectors along the [001]_tilted, [011]_tilted, and [111]_tilted are (0, $\sin 2^\circ$, $\cos 2^\circ$), (0, $\sin 47^\circ$, $\cos 43^\circ$), and ($\sin 57^\circ \cos 45^\circ$, $\sin 57^\circ \sin 45^\circ$, $\cos 53^\circ$), respectively.

Figure 1. Configurations of (a) C as PKA in ZrC crystal, (b) Zr as PKA in ZrC crystal, (c) C as PKA in ZrC with one C vacancy, and (d) Zr as PKA in ZrC with one C vacancy. The high-symmetry crystallographic directions of displacement are labeled with the atom and direction of displacement. For example, C[001] means to displace C atom along the [001] direction.

In the third step in the AIMD simulations, for the initial kinetic energies around the estimate E_d from step two, longer time simulations with a time step of 1fs with a thermostat at 300K are performed for the evolution of produced defects (the evolution runs). The stability of Frenkel pairs is tested for about 3 ps. If a stable Frenkel pair is formed in AIMD simulations, the system is then subsequently relaxed at 0K to reach the stable configuration to ensure that the Frenkel pair is stable. To determine E_d , simulations are performed for each kinetic energy (E_k) value given to the PKA atom and E_d is set at the lowest value where a Frenkel pair is formed.

Initially all three steps are performed for each case on a coarse grid of energies with an energy interval of 5 eV in order to approximately determine E_d , which requires at most 10 simulations (one at each E_k value). Then about five runs with an energy interval of 1 eV around the approximate E_d determined from the coarse grid are conducted to improve the precision so that the value where the Frenkel pair is formed is accurate to within 1 eV. Once the value for E_d is known, a final longer time AIMD simulation (for about 1ps) is checked to make sure the Frenkel pair is stable. This 1 eV range of possible values is then used as the estimated errors bars in Tables 1 and 2.

3. Results and Discussion

3.1. E_d for impulses along the high-symmetry crystallographic directions

Table 1. Threshold displacement energies in ZrC and SiC (SiC from Ref.[14]), along the high-symmetry crystallographic directions (the $[\bar{1}\bar{1}\bar{1}]$ direction is equivalent to the $[111]$ direction in ZrC). The heading “Defect” refers to the final Frenkel pair defect structure formed. V_C and V_{Zr} are a C vacancy and Zr vacancy, respectively. Zr_{Td} is a Zr interstitial located in a Zr-centered double tetrahedron. d_{FP} is the distance between the interstitial (the middle C atom of the C-C-C trimer, or closer Zr atom of the Zr-Zr dumbbell) and the vacancy of the Frenkel pair. The error bar of 1 eV is determined as described in Section 2.

Direction	E_d in ZrC (eV) 216 atoms	E_d in SiC (eV) 1000 atoms[14]	Defect	d_{FP} (a_0)
C[001]	19±1	20.0	V_C +C-C-C trimer	0.47
C[011]	20±1	22.5	V_C +C-C-C trimer	0.47
C[111]	7±1	20.5	V_C +C-C-C trimer	0.47
C $[\bar{1}\bar{1}\bar{1}]$	7±1	47.5	V_C +C-C-C trimer	0.47
C sublattice weighted average	16±1	25.5		
Zr[001]	71±1	49.5	V_{Zr} +Zr-Zr dumbbell & 2 V_C +C-C-C trimer + C-C dumbbell	0.82
Zr[011]	22±1	70.0	V_{Zr} +Zr-Zr dumbbell	1.20
Zr[111]	33±1	105.0	V_{Zr} + Zr_{Td} & V_C +C-C-C trimer	0.81

Zr $[\bar{1}\bar{1}\bar{1}]$	33 $\pm$ 1	62.0	$V_{\text{Zr}+\text{Zr}_{\text{Td}}} \& V_{\text{C}+\text{C}-\text{C}-\text{C}} \text{ trimer}$	0.81
Zr sublattice weighted average	37 $\pm$ 1	69.4		

Table 1 and Fig. 2 report the results of E_d of C and Zr atoms along the main high-symmetry crystallographic directions in ZrC. Results for SiC [12, 14] are also included for comparison. We include directions $[111]$ and $[\bar{1}\bar{1}\bar{1}]$ as they are different in SiC, although they are equivalent for ZrC. We note that as the structures of ZrC and SiC are rocksalt and zincblend, respectively, the different directions do not correspond to the same environments. Therefore, differences in E_d between the two systems may be due to both their different chemistries and their different structures, and any interpretation of the origin of these differences must at least take both possibilities into account. It is shown that E_d is strongly anisotropic. It is easiest to displace C atom along the $[111]$ direction ($E_d(\text{C}[111]) \approx 7 \pm 1$ eV) and most difficult along the $[011]$ direction ($E_d(\text{C}[011]) \approx 20 \pm 1$ eV). This ordering can be rationalized in terms of the structure and chemistry of ZrC. In particular, the low value along the $[111]$ direction can be explained by the fact that when the C PKA was displaced along this direction it moves into a region of significant open space and rapidly begins to form bonds with the second nearest-neighbor C atoms before colliding with the third nearest-neighbor Zr atom. This bonding effect, which stabilizes the $[111]$ direction, does not occur in the other directions. Along the $[011]$ direction, the

C PKA kicks out its second nearest neighbor C atom along the [011] direction, the C PKA goes back to its original lattice site, and the kicked-out C atom forms a C-C dumbbell with the sixth nearest neighbor C atom of the original PKA site. Along the [001] direction ($E_d(\text{C}[001]) \approx 19 \pm 1$ eV), the C PKA impacts a Zr atom, which rebounds the C atom backward due to the much greater mass of Zr. The returning C atom passes near its original lattice site, and then it deviates further from the lattice site while it vibrates back and forth. Eventually, this C atom becomes a C interstitial and diffuses to its neighboring atoms and forms a stable C Frenkel pair.

The average E_d values reported in Table 1 correspond to the weighted average calculated over the four high-symmetry directions. The weighting factors take into account the number of physically distinct but symmetry equivalent directions in ZrC, which are 6 for [001], 12 for [011], 4 for [111] and 4 for $[\bar{1}\bar{1}\bar{1}]$. For the C PKA, the weighted average value of E_d is 16 ± 1 eV. For all cases of C displacement, C Frenkel pairs rather than Zr Frenkel pairs are formed at the end of the MD simulation, presumably in part due to the fact that the C PKA is displaced most dramatically, and perhaps in part due to the much lower formation energies of C Frenkel pairs than Zr ones[3, 7]. The C Frenkel pairs at the end of MD runs are fully relaxed to obtain their stable configuration. The C interstitial (the C-C-C trimer) is not far from the C vacancy site. The interstitial-vacancy separation d_{FP} , which is defined as the distance from the C interstitial atom at the middle of the C-C-C trimer to the vacancy lattice site (i.e., the position that the C

occupied before it was removed), is about $0.47 a_0$, where $a_0 = 4.72 \text{ \AA}$ is the lattice constant of ZrC unit cell.

For the Zr atom, the easiest direction to displace the atom is along the [011] direction ($E_d(\text{Zr}[011]) \approx 22 \pm 1 \text{ eV}$), while the hardest direction is along the [001] direction ($E_d(\text{Zr}[001]) \approx 71 \pm 1 \text{ eV}$). In the [011] direction, the Zr PKA kicks out its second nearest-neighbor Zr atom and replaces it. After fully relaxation, a stable Zr FP with the interstitial-vacancy separation $d_{\text{FP}} \approx 1.20a_0$ is formed (the distance is measured from the closer Zr of the Zr-Zr dumbbell to the Zr vacancy site). Along the [001] direction, the Zr PKA kicks out its first nearest-neighbor C atom, which forms a C-C dumbbell. Then the Zr PKA forms a Zr-Zr dumbbell and kicks out another C atom which forms a C-C-C trimer. Thus one Zr FP with $d_{\text{FP}} \approx 0.82a_0$ and two additional C FPs are formed. In the [111] direction ($E_d(\text{Zr}[111]) \approx 33 \pm 1 \text{ eV}$) the displaced Zr PKA kicks out its third nearest-neighbor C atom, which forms a C-C-C trimer. The Zr PKA moves to the interstitial site of Zr-centered double tetrahedron. After fully relaxation, a stable Zr FP with the interstitial-vacancy separation $d_{\text{FP}} \approx 0.81a_0$ is formed.

To explore the possible correlation between the amorphization resistance and E_d , we compare our calculated E_d in ZrC with E_d in SiC, determined using similar AIMD methods in Ref. [12]. These two systems might show important differences as ZrC has much higher amorphization resistance than SiC [8]. As shown in Table 1 and Fig. 2, the averaged E_d values on Si and C sublattices are about 25.5 eV and 69.4 eV, respectively,

compared to 16 ± 1 eV and 37 ± 1 eV on the Zr and C sublattices. Thus the values of E_d are actually lower in ZrC than those in SiC (especially along the directions $C[\bar{1}\bar{1}\bar{1}]$, $Zr/Si[011]$ and $Zr/Si[111]$), despite the greater resistance to amorphization of ZrC. These results indicate that the values of E_d have little to do with the fact that SiC can be readily amorphized [29-32] while ZrC cannot [8].

Figure 2. The comparison of E_d values on the C and Zr(Si) sublattices in ZrC (blue) and that in SiC (red), along each of the high-symmetry crystallographic directions as well as the weighted average sublattice values. SiC values are from Ref.[14].

3.2. E_d for impulses just off the high-symmetry crystallographic directions

Since E_d values are highly anisotropic, we now check the dependence of E_d on tilting by a small angle off the high-symmetry crystallographic directions. Comparing E_d along the exact crystallographic directions with those along the corresponding tilted directions, the energy changes are within the uncertainty range of 1eV, as shown in Table

2. The overall small differences indicate that there is no obvious effect on E_d by slightly tilting the PKA velocity direction off the high-symmetry crystallographic directions. This is expected from the fact that the PKA atom vibrates around its lattice site at room temperature, which already breaks any symmetry of the PKA atom displacement. Therefore, there is no significant difference between the impulse direction along the high-symmetry crystallographic direction or slightly off this direction.

Table 2. Threshold displacement energies for ZrC along the exact or tilted high-symmetry crystallographic directions and with a C vacancy (V_C). The error bar of 1 eV is determined as described in Section 2.

Direction	E_d perfect (eV)	E_{d_tilted} perfect (eV)	E_d with V_C (eV)
C[001]	19±1	19±1	20±1
C[011]	20±1	21±1	21±1
C[111]	7±1	7±1	11±1
C sublattice weighted average	16±1	16±1	18±1
Zr[001]	71±1	72±1	71±1
Zr[011]	22±1	21±1	21±1
Zr[111]	33±1	34±1	34±1
Zr sublattice weighted average	37±1	37±1	37±1

3.3. E_d in the presence of C vacancies

Considering that ZrC_x can be stable with a wide-range of sub-stoichiometries ($0.6 < x < 0.98$)[2], it is important to consider the effect of C vacancies (V_C) on the threshold displacement energies. To explore the effect of V_C , initial structures were created with a V_C as the nearest-neighbor of a C PKA along the [011] direction and as the nearest-neighbor of a Zr PKA along the [001] direction, as shown in Figs. 1 (c) and (d). The E_d values for C and Zr along the high-symmetry directions in the presence of the V_C are shown in Table 2. The largest change is increase in E_d in C[111] by 4 eV. Other changes are within the error range. The biggest change is found in the case of C[111] with V_C because the low E_d value for this case was in part due to a bonding of the PKA C with nearest neighbors (see Sec. 3.1). The V_C therefore reduces opportunities for this bonding, and increases E_d by about 4 eV to 11 ± 1 eV.

Figure 3. The E_d values in ZrC for the three cases studied in this work: (i) E_d for impulses along the high-symmetry crystallographic directions in the perfect crystals (E_d perfect,

blue); (ii) E_d for impulses tilted off the high-symmetry crystallographic directions in the perfect crystals (E_d _tilted perfect, red); (iii) E_d for impulses along the high-symmetry crystallographic directions in ZrC in the presence of a C vacancy near the PKA (E_d with V_C , green).

As a summary, Fig. 3 shows the comparison of our results for the three cases studied in this work, (i) E_d along the high-symmetry directions in the perfect crystal, (ii) E_d along the slightly-off high-symmetry directions in the perfect crystal, and (iii) E_d along the high-symmetry directions in the presence of V_C . The weighted average E_d values along the slightly-off high-symmetry directions or in the presence of V_C are equal to the corresponding value along the high-symmetry directions in the perfect crystal for Zr, and differ slightly for C for in the presence of V_C due to the change in C[111] in the presence of V_C .

4. Conclusion

We used ab initio molecular dynamics (AIMD) methods to calculate E_d in ZrC along the main crystallographic directions, tilted directions, and in the presence of a C vacancy. The averaged threshold displacement energies along the main crystallographic directions on the C and Zr sublattices are 16 eV and 37 eV, respectively. Our average E_d results are smaller than the estimated average E_d of 25 eV for C and similar to the E_d of

35 eV for Zr reported by Gosset, et al. [5], which were estimated indirectly based on values measured in TaC. We expect that these first principles calculations of E_d in ZrC will provide a more reliable estimation than this simple extrapolation. In addition, our calculations provide detailed insight into the Frenkel pair formation mechanisms and directional dependence of E_d in ZrC.

The sensitivity of E_d on the directions was investigated by tilting the directions of PKA velocities from the main crystallographic directions by a small angle. No obvious effects were found. A neighboring C vacancy can increase the values of E_d , although the effect was just 4 eV and only along a specific direction.

Our results provide an understanding of the basic damage production processes in ZrC. Furthermore, they provide a foundation for aiding the design and interpretation of ZrC irradiation experiments and support for irradiation modeling, e.g., for use in validating potentials or input to SRIM simulations.

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Appendix

In the literature there are sometimes different definitions for the threshold displacement energies [12-15]. In this paper, E_d is defined as the minimum energy required to permanently displace the same type of atom as the PKA [13-15], which we believe is the most widely used definition. Another possible definition is to define the threshold displacement energy as the minimum energy required to form a stable Frenkel pair of any type, i.e., the Frenkel pair may or may not be on the same type of lattice as the PKA [12]. We denote this alternative definition as E_d' . For completeness Table A.1 lists E_d' values in ZrC and SiC[12] using this alternative definition.

Direction	E_d' in ZrC (eV) 216 atoms	E_d' in ZrC (eV) 64 atoms	E_d' in SiC (eV) 64 atoms[12]
C[001]	19±1	20±1	18±1
C[011]	20±1	17±1	14±1
C[111]	7±1	39±1	38±1
C[$\bar{1}\bar{1}\bar{1}$]	7±1	39±1	38±1
C sublattice weighted average	16±1	22±1	19±1

Zr[001]	18±1	33±1	46±1
Zr[011]	22±1	22±1	45±1
Zr[111]	27±1	32±1	22±1
Zr[$\bar{1}\bar{1}\bar{1}$]	27±1	32±1	22±1
Zr sublattice weighted average	22±1	27±1	38±1

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