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COMMENT

Comment on 'Large swelling and percolation in irradiated zircon'

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Abstract

A recent model for the large radiation-induced swelling exhibited by irradiated zircon ($ZrSiO_4$) is partially based on results of molecular dynamics (MD) simulations of the partial overlap of two collision cascades that predict a densified boundary of polymerized silica and the scattering of the second cascade away from the densified boundary (Trachenko *et al* 2003 *J. Phys.: Condens. Matter* **15** L1). These MD simulations are based on an atomic interaction potential for zircon (Trachenko *et al* 2001 *J. Phys.: Condens. Matter* **13** 1947), which, according to our analysis, only reproduces some of the crystallographic properties at equilibrium and does not adequately describe the atomic scattering physics for zircon, and on simulation methodologies for energetic events that are ill defined. In fact, the interatomic potential model used by Trachenko *et al* yields a significantly more rigid structure, with very high Frenkel defect formation energies and extremely low entropy and specific heat capacity. Consequently, the reported results of the cascade simulations, which are events far from equilibrium, may be artifacts of both the potential model and simulation methodologies employed. Thus, the structural changes predicted by the simulations must be viewed cautiously, as these simulation results cannot be taken as confirmation of a new scattering physics process that is the basis for the proposed swelling model. In this comment, the deficiencies in the atomic interaction potential and methodologies employed by these authors are critically reviewed, and the validity of the cascade overlap simulations and proposed physics is discussed.

Introduction

Trachenko *et al* [1] recently presented a letter proposing a new model for describing the large radiation-induced swelling in zircon ($ZrSiO_4$). This new model is partially based on and justified by the results of molecular dynamics (MD) simulations of 30 and 70 keV energetic displacement cascades [2, 3] that show the formation of a densified boundary of polymerized silica about a single cascade; furthermore, the partial overlap of a second cascade event with the first cascade results in the scattering of the energy transfer processes off the densified boundary of the first cascade. The process of scattering a second cascade off the boundary of an existing cascade is proposed as the driving force for the large swelling observed in zircon that is described by a percolation theory model. In this comment, we show

(1) that the atomic interaction potential derived for zircon by Trachenko *et al* [3] is deficient in predicting key thermodynamic, mechanical, and chemical properties;
(2) that the cell sizes used in the simulations are inconsistent with expected behaviour;
(3) that there are issues with the simulation methodology that could bias the results; and
(4) the results are inconsistent with experiment.

Our analysis is based on the essential properties that atomic interaction potentials must predict and the simulation methodologies that must be followed to study radiation damage processes in ceramic oxides [4].

1. The interaction potential

As a means to understand the effects of alpha decay on the structure of zircon, Trachenko *et al* [1, 2] used MD methods to simulate the evolution of structural changes due to the energetic collision cascades that are initiated by imparting kinetic energy to a Zr atom. The force field used to describe the interactions of all atoms included pair and three-body potentials, which was claimed to provide a reasonable description of the equilibrium structure of zircon [3]. Unfortunately, these authors only validated their potential against lattice parameters, bond lengths, and bond angles (i.e., atomic positions) in the zircon structure, which as reported yields a reasonable structure, and did not provide a check of the mechanical and thermodynamic properties, as well as defect formation energies and relaxation processes in zircon. Without further evaluation of the potential and the properties that control kinetic energy dissipation, the validity of simulations of energetic cascades that take the system far from equilibrium is highly suspect. The mechanical and thermodynamic properties, as well as the Frenkel defect formation energies, were determined using the GULP code [5] with the interaction potential model parameters described in [3]. These physical properties are absolutely necessary to validate the potential model, not only because experimental data exist, but more importantly because these properties govern the manner in which the energy is dissipated and absorbed in zircon during the energetic collision cascades. Table 1 provides a summary of results determined by us, those reported in [3], and those obtained from experiment and first-principles calculations [12]. The parameter used for the three-body O–Si–O interaction was not reported in [3] and, thus, that of Sanders *et al* [6] was used. Note that in the Sanders *et al* formalism the three-body term is given by $E_{ijk} = K(\theta - \theta_0)^2$, whereas both the GULP [5] and DLPOLY [7] (used in [3] to carry out the simulations) codes use the formula $E_{jik} = (K/2)(\theta - \theta_0)^2$. However, this parameter has no particular influence on the main argument of this paper, since the lattice geometries and the mechanical and thermodynamic properties are nearly identical in the two cases.

A careful comparison of properties determined using the Trachenko *et al* potential with those obtained by experiment is informative. The bulk modulus and the entropy reveal a

Table 1. Properties of zircon determined by the GULP code using the Trachenko *et al* force field [3] as compared to those determined by experiment and first-principles calculations [11] for Frenkel pairs and those also published in [3]. GULP (1) is with $K = 2.907$ eV deg^{-2} and GULP (2) is with $K = 4.194$ eV deg^{-2}.

	Experiment	GULP (1)	GULP (2)	Trachenko *et al*
Unit-cell parameters (Å)				
a, b	6.604	6.520	6.553	6.520
c	5.979	6.096	6.035	6.095
Bond lengths (Å)				
Si–O	1.623	1.545	1.541	1.614
Zr–O1	2.128	2.204	2.203	2.137
Zr–O2	2.267	2.251	2.258	2.231
Bond angles etc				
O–Si–O (1) (deg)	976	91	93	95
O–Si–O (2) (deg)	116	120	118	117
Unit-cell volume (Å^3)	130.6	129.6	129.6	Not reported
Bulk modulus (GPa)	225.2	531.5	583.3	Not reported
Elastic constants (10^{11} dyn cm^{-2})				
C_{11}	42.4	118.8	122.2	Not reported
C_{33}	49.0	127.6	128.1	Not reported
C_{44}	11.4	13.7	13.6	Not reported
C_{66}	4.85	1.83	2.42	Not reported
C_{12}	7.03	12.7	13.9	Not reported
C_{13}	14.9	35.2	32.3	Not reported
Heat capacity				
C_v (300 K) (J mol^{-1} K^{-1})	98.6	65.1	64.4	Not reported
Entropy				
S (300 K) (J mol^{-1} K^{-1})	84.4	43.3	42.6	Not reported
Frenkel pairs (eV)				
O (DFT/LDA)	7.3	16.9	18.7	Not reported
Zr (DFT/LDA)	24.0	55.4	57.9	Not reported
Si (DFT/LDA)	22.9	58.9	62.7	Not reported

simulated zircon structure that is almost three times harder than the actual structure described by the experimental modulus, with a vibrational entropy that is a factor of two lower than the experimental value. Consistent with this observation, the elastic constants are also significantly higher than the experimentally determined values. Finally, the formation energies of the extended Frenkel pairs are twice as high compared to those calculated by first-principles calculations [12]. As a result, this potential only describes the crystallographic properties at equilibrium and is incapable of reproducing any other physical property of zircon. Conversely, it leads to a much stiffer material than the actual zircon structure, which results in more energy being absorbed locally in the displacement of atoms and formation of defects. In addition, the heat capacity, C_p, is very low; hence the temperature can increase rapidly at low energy cost. However, we cannot know what the final influence of the thermal effects in these simulations is without knowing the heat conductivity of Trachenko's model, and how the velocities were scaled in the system during the cascade simulations (see the comments below).

Another critical feature of any potential model used in MD simulations of collision cascades is that the short-range interactions must correctly describe the atomic scattering physics for all atoms in the structure. The Buckingham potential has a pathology at small distances where the r^{-6} term dominates over the exponential term. Trachenko *et al* [2, 3] incorporated a short-range repulsive potential to amend the pathology that occurs only for their Si–O and O–O potentials. Unfortunately, these authors do not provide any description of the short-range potential employed or a physical basis for the choice, but it can be assumed that it provides an adequate fix. In figure 1, we have shown a possible correction using a functional form of

$$E_{\mathrm{corr}} = 4d_{ij}\left\{\left(\frac{e_{ij}}{r_{ij}}\right)^{24} - \left(\frac{e_{ij}}{r_{ij}}\right)^{6}\right\},$$

with $d_{\mathrm{OO}} = 0.0075$ eV, $e_{\mathrm{OO}} = 1.20$ Å, $d_{\mathrm{SiO}} = 0.000\,2278$ eV, and $e_{\mathrm{SiO}} = 1.20$ Å. The choice of this correction is generally considered to be arbitrary for the case of acquiring data at equilibrium. But for collision cascades, it is general practice to describe the short-range interactions of energetic atoms by using short-range repulsive potentials based on *ab initio* calculations, as in the case of SiC [8, 9], or to use the well established Ziegler–Biersack–Littmark (ZBL) screened Coulomb potential [10], as in MD studies on zircon by other groups [11–13] and numerous simulations of energetic cascades in metals and semiconductors [14–17]. The screened ZBL potential provides a reasonably accurate description of the nuclear stopping power, atomic scattering cross sections, and energy dissipated by elastic scattering collisions as demonstrated by consistent agreement with experimental measurements of both scattering cross sections and energetic particle ranges in a wide variety of solids [10]. Consequently, it is often used as a benchmark for a potential's ability to describe the short-range interactions in MD simulations of ion–solid interactions. To determine the adequacy of the total potential for describing the collision and scattering physics, which determines the range of the 30 and 70 keV Zr ions, as well as the extent of the defect and recoil distribution, we compare the Trachenko *et al* potential interactions (with and without the correction at small r) for Si–O and O–O directly with the corresponding ZBL potentials in figure 1. Also shown are the same potential curves for the Zr–O interactions, but where the Buckingham potential has no contributions from the r^{-6} term, and so no correction is necessary. The significant deviations of the atomic scattering cross sections are illustrated in figure 1. In addition, the cation–cation interactions also require a modification to correct for the scattering cross section. Using only the Coulomb repulsive energy leads to identical short-range interactions for the Si and Zr cation pairs when a rigid ion model is used, because these ions have identical charge. In figure 2, we show the Coulomb energy for a pair of 4+ valence ions and include the ZBL potentials for the Zr–Zr, Zr–Si, and Si–Si interactions. In summary, the Si–O and O–O modified short-range interactions can be chosen to be in close agreement with the ZBL interactions, although slopes at high energy are of concern. The correction chosen by us shows too steep a slope for the hard-wall with respect to the ZBL potential, whereas other choices for the correction can be less steep. Thus a direct fit to the ZBL potential would be best. In contrast, the Zr–O interactions reveal cross sections that are about a factor of four too large, relative to the ZBL cross sections, whereas the cation–cation interactions reveal cross sections that are too small for all pairs. Given that the system is dominated by the presence of O atoms, the majority of the initial Zr recoil energy will be transferred in Zr–O collisions, thus excessively scattering the O atoms, with the lighter Si cations being dragged along by the dominant Coulomb forces. On another note, regarding the treatment of Coulomb interactions by Trachenko *et al*, it was never specified how they treated the long-range interactions: i.e., did they truncate the potential, and if so at what cut-off; or did they use Ewald sums, and if so what were the parameters?

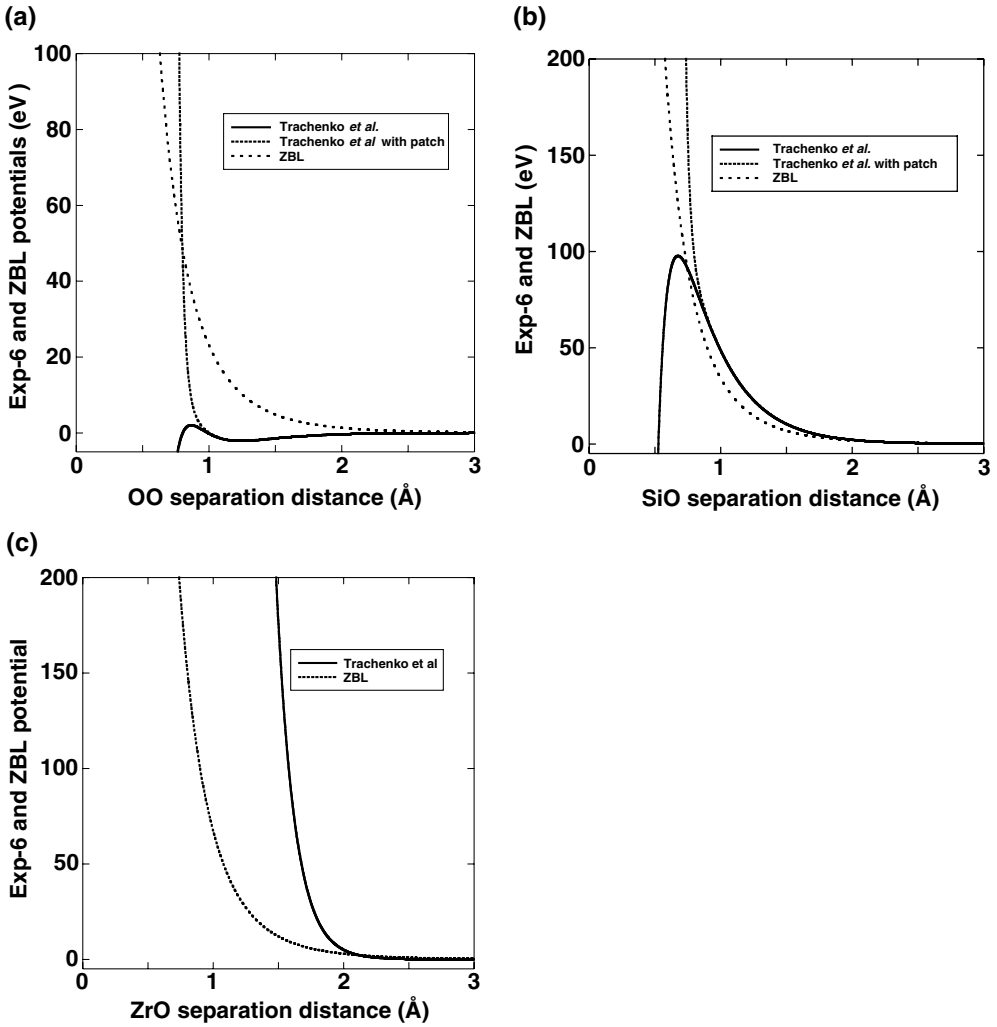

Figure 1. A comparison of the Buckingham potential of Trachenko *et al* and the ZBL interactions for (a) O–O, (b) Si–O, and (c) Zr–O ion pair interactions. A possible short-range repulsive correction (see the text) is included; note that the Zr–O interaction has no r^{-6} term.

2. Simulation cell sizes and the extent of cascades

In their MD simulations, Trachenko *et al* [1, 2] simulated the collision events associated with imparting 30 or 70 keV to Zr atoms. An easy test of the adequacy of the short-range repulsive potential is to compare the projected range of the particles in the simulation with the projected range based on the ZBL potential. This can be easily carried out using the SRIM (stopping and range of ions in matter) code [10, 18], which uses a Monte Carlo binary collision approximation based on the ZBL potential to describe elastic scattering. The SRIM code also includes the electronic stopping power as an energy loss mechanism. Since most MD simulations of ion–solid interactions, including those of Trachenko *et al* [1–3], do not include electronic energy loss processes because of added computational complexity, a modified version of the SRIM code has been used that will calculate particle ranges and the distribution of recoils, defects, and

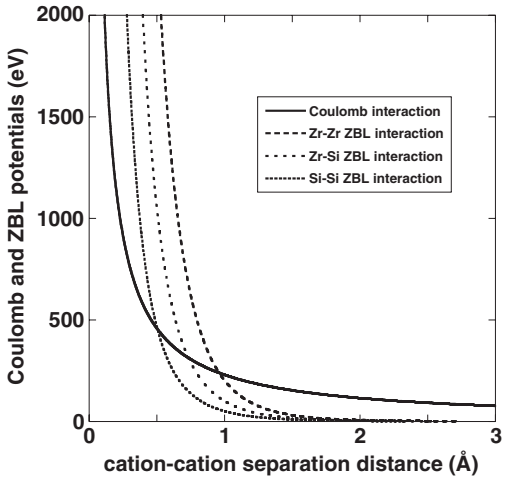

Figure 2. Comparison of the Coulomb interaction of cation pairs each with a 4+ valence charge and corresponding ZBL interactions for the cation pairs.

Table 2. The average longitudinal and lateral radial ranges for energetic Zr and U atoms and the minimum tetragonal volume needed to contain the cascade. The calculations are based only on nuclear stopping processes defined by the ZBL potential.

Recoil	Longitudinal (nm)	Lateral radial (nm)	Minimum volume (nm^3)	Minimum volume (atoms)
1 keV Zr	2.1	0.9	7	644
30 keV Zr	15.2	5.9	2 116	194 713
70 keV Zr	29.0	10.9	13 782	1267 940
5 keV U	5.6	1.7	65	5 980

energy dissipation based only on the screened ZBL potential. Because the electronic energy loss mechanisms are not included in the modified SRIM code, the particle ranges are longer while the recoil distributions and energy dissipation are more disperse than with the original SRIM code, but this provides a more accurate description of the behaviour expected in the MD simulations. Using the modified SRIM code, we have calculated the longitudinal range and lateral dispersion for 30 and 70 keV Zr recoils in zircon, which define the minimum tetragonal MD cell volume needed to just contain an average cascade (50% of the cascades will exceed the cell volume). The results are given in table 2. Also included in table 2 are the results for a 1 keV Zr recoil, that can be compared with the simulation performed by Devanathan *et al* [13] in zircon using an MD cell containing 5184 atoms, and the results for a 5 keV U recoil in zircon, that can be compared with the simulations performed by Crocombette and Ghaleb [12] using an MD cell containing 139 968 atoms.

If a more realistic potential and temperature scaling were to be used, the cell sizes selected by Trachenko *et al* [1, 3] should be too small to avoid cell size effects. It has been long established in the field of MD simulations of radiation effects in materials that the MD cell size needs to be quite large to avoid cell size effects. An empirical relationship developed by Foreman *et al* [19] for metals recommends that the number of atoms in the cell should be about 16 times the recoil energy in electronvolts, and this relationship is often used to determine the adequate cell size for metals. This relationship would suggest that the number of atoms in

the MD cells for 30 and 70 keV Zr recoils should contain 480 000 atoms and 1120 000 atoms, respectively; however, the cell size predicted for 70 keV Zr is smaller than the minimum volume indicated in table 2 to completely contain 50% of the cascades. A better criterion for ionic-bonded materials, such as zircon in which the significant differences in constituent masses leads to more highly dispersed cascades than in metals, might be cell sizes that are about an order of magnitude larger than the minimum volume (table 2) needed to contain an average cascade, as was the case in the studies of Devanathan *et al* [13] for Zr energies up to 1.0 keV and Crocombette and Ghaleb [12] for 5.0 keV U. In support of much larger cell sizes for energetic recoils of the magnitude used in the studies of Trachenko *et al* [1, 2], MD simulations of 30 and 50 keV Si recoils in silicon carbide required MD cell sizes of 2000 000 atoms and 6000 000 atoms, respectively, to contain the cascades [9, 20].

Trachenko *et al* [1, 2] employed MD cells containing 192 000 and 375 000 atoms for the 30 and 70 keV Zr recoils, respectively. Comparing with the results in table 2, the MD cell employed for the 30 keV Zr recoils should be just large enough to contain less than 50% of the cascades. There is an even greater disparity in the MD cell employed for the 70 keV Zr recoils. The probability of containing a 70 keV Zr recoil cascade in a cell of this small size using appropriate short-range repulsive potentials should be very low, if appropriate thermostat controls are applied. The facts that Trachenko *et al* [1, 2] readily contained the Zr recoils in their cells and did not detect finite size *effects* indicate that the short-range repulsive potentials coupled to an extremely stiff structure model, along with questionable temperature scaling, do not correctly describe the elastic scattering physics and propagation of energy transfer for all the atoms in zircon. This is dramatically demonstrated by the their estimate that damage for a 70 keV Zr recoil is contained within a sphere of radius 3.5 nm [2], despite the fact that the average range for a 70 keV Zr recoil in zircon should be about 29 nm (table 2) based on elastic scattering interactions only. The result is that the short-range interactions and temperature scaling used by Trachenko *et al* significantly increase the local energy deposition, atomic displacements, and ballistic mixing. Without more details on the short-range potential employed, the spatial extent of the cascades generated and the methodologies used, we cannot determine how, and to what extent, these MD simulations may have overestimated the local damage production. Considering the difference in damage volume or the size of the MD cell employed for the 70 keV Zr cascade versus the minimum volume needed to contain a more realistic average cascade (table 2), it must be concluded that the local energy deposition is overestimated by at least a factor of four, which may be largely attributed to the nearly factor of four increase in the Zr–O scattering cross sections.

3. Simulation methods and temperature scaling

Simulation methodologies are well established for the study of collision cascades using atomic interaction potentials [14–17, 21]. These methods are designed to allow a simulated system to evolve as far and as long as possible without interference of external controls, such as temperature regulation. External controls are used because simulations carried out with periodic boundary conditions can allow excess energy in the form of a thermal dissipation or mechanical shock wave to exit the primary image cell through a boundary edge and consequently re-enter the primary image cell through the corresponding boundary. *Finite size* effects, important to displacement cascade simulations, consist of processes that carry excess kinetic energy across a boundary. Large simulation boxes can significantly reduce such effects, but also the excess energy can be controlled by absorbing boundaries to minimize interference when box sizes are small and the energy of the primary knock-on atom (PKA) is large. Thus, in practice two things are generally done: one is to match the energy of the PKA

to the cell size following a general rule (see above) and the second is to apply energy absorbing controls only at the boundaries with some well defined thickness. Particular advantage can be taken of the shape of the primary cell and of the fact that the PKA and its thermal and shock waves have a certain amount of directionality to them. However, there is still an upper limit to the energy that a cell can absorb. In removing energy, it is more realistic that the energy, whether thermal or mechanical, be removed at a rate that follows the bulk behaviour of the simulated system, which preferably matches the properties of the real system [22].

In the original work of Trachenko *et al* [3], the simulation technique employed did not adhere to the above requirements. Although it is somewhat vague in its published representation the simulations were apparently carried out using a standard temperature scaling technique that uniformly removes excess energy from the entire system. This can lead to artificial quenching of the dynamics behaviour and response of the system prematurely. It is possible that this is not a core problem in those simulations because in applying a temperature scaling technique usually the kinetic energy rescaling occurs at time intervals anywhere from 5 to 100 time steps apart, in between running basically as an NVE ensemble. Neither the rate of temperature scaling nor the algorithm employed were reported, and so it is difficult to evaluate whether the scaling procedure interfered or not. It is even more difficult to duplicate their constant stress simulations because the algorithm choices and parameters were not published. Studies have shown that for large system sizes at appropriate PKA energies, the NVE ensemble without absorbing or attenuating boundaries works [23], but is expected to break down as the PKA energy is increased while maintaining the same system size. In a PKA simulation within an NVE ensemble, the temperature of the system increases significantly and only a small of amount of excess kinetic energy is observed to cross the boundary [24]. It has been shown that a consistent approach for removing heat consistent with the NVE ensemble is to use kinetic energy attenuating boundaries [23]. Temperature control is vital in creating overlapping cascades since the system must be at thermal equilibrium at some specified temperature before another displacement cascade is introduced. Thus, temperature control must be carried out at the end of a cascade simulation as with a simulation carried out with NVE ensembles, or the energy must be attenuated at the boundaries.

4. Validity of results

Another very important concern is related to drawing direct comparisons between these simulation results and the experimental data. In the natural zircons used to validate the findings of the MD simulations, alpha decay of the U and Th impurities produces an energetic alpha particle (4.0–4.6 MeV) and a lower-energy (69–78 keV) Ra or Th recoil nucleus. The recoil nuclei are much heavier than the Zr PKA used in the simulations. The partitionings of energy between nuclear and electronic stopping will be dramatically different. (Note that classical simulations do not account for electronic stopping processes, important to these types of simulation [25]. This is a shortcoming of classical potentials for zircon and available methodologies, as discussed elsewhere [4]. The validity and appropriateness of the classical simulations lies in their ability to correctly describe the elastic energy transfer.) The elastic energy transfer, as well as the electronic relaxation and charge exchange, of the Ra or Th recoil colliding with Zr, Si, and O atoms will likewise be significantly different to that from the Zr PKA to Zr, Si, and O, leading to significantly different distributions of energy transfer, defect formation, and lattice restructuring. Such differences between O, Si, and Zr projectiles have been observed in previous simulations [26]. Furthermore, only about 50% of the Th and Ra recoil energy in natural zircons is dissipated in nuclear collisions (i.e., damage energy); the rest is dissipated by electronic energy loss. Thus, the damage energy from the Ra or Th recoils

in actual zircon is of the order of 35 keV and is dissipated over the 20–25 nm range of the Ra and Th recoils. In what is claimed by Trachenko *et al* to be the most realistic simulation description, 70 keV of damage energy is dissipated over a range of about 5–7 nm, which is in significant contrast to the results in table 2 and the ranges for Ra and Th recoils. Thus, it can only be considered fortuitous that the size of the 70 keV Zr cascade is consistent with some experiments for amorphous domain sizes (5 nm diameter) in natural zircon, where the actual cascade sizes are considerably larger. Furthermore, since the simulation timescales are of the order of 10 ps, the final state issued from the simulations cannot directly be compared with those observed in natural zircons since the thermal evolution is completely ignored.

5. Conclusions

These analyses raise questions about the validity of the structural changes predicted by the MD simulations performed by Trachenko *et al* [1, 2]. The collision cascade and resulting defects and structural changes should be more dispersed than predicted by the simulations. The polymerization of SiO_n polyhedra predicted by their MD simulations have also been observed, but to a much lesser extent, in the MD simulations of Devanathan *et al* [13] and Crocombette and Ghaleb [12] and by NMR experiments [27] on natural zircons damaged by alpha decay events over geologic timescales. Consequently, the MD simulations of Trachenko *et al* [1, 2] may not correctly predict the mechanism and degree of such polymerization, and the observed results may be an artifact of their potential and methodology. While we would like to perform MD simulations of 30 keV Zr recoils in zircon using what we believe are more realistic potentials, which include the ZBL potential for the short-range interactions, the necessary MD cell would need to contain about 2000 000 atoms, which is currently computationally too costly, even with the use of cut-offs for the Coulomb interactions.

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