DYNAMIC SIMULATION OF RADIATION DAMAGE IN ZIRCON DUE TO NUCLEAR WASTE LOADING

M. H. Hassan

Nuclear Engineering Department,
Alexandria University, Alexandria, Egypt

ABSTRACT

Zircons, which are hundreds of millions of years old, experience a transition from the crystalline state (<10^{23} alpha-disintegrations/m^3) to the amorphous state (> 10^{26} alpha-decays/m^3). Compositional changes were predicted to have an impact on nuclear waste material behavior resulting in changes like local swelling. Recent experiments identified the presence of zirconium- and silicon-rich domains, which are less than 10 Å in size. At high doses, changes in atomic concentrations in the host matrix should be taken into consideration necessitating the use of dynamic simulation of the target. Also, the effects of electronic energy deposition on the physical properties of the matrix as a function of doses are highly needed. In previous ion irradiation simulation in zircon, only thin samples were used. This configuration does not allow the probing of the impact of nuclear atomic displacements and the subsequent atomic mixing on the compositional changes, especially at the end of the alpha track. Ne (0.8 MeV), Ar (1.5 MeV), Kr (1.5 MeV), and Pb (230 keV) simulations were done for 10^{15} ions/cm^2. Also, 4.5 MeV alpha irradiations were simulated for 10^{15}, 10^{18} and 10^{20} He ions/cm^2 representing different loading of nuclear waste materials. Electronic energy loss was properly assessed.

Keywords: Dynamic simulation, Radiation damage, Zircon, Nuclear waste

INTRODUCTION

Radiation damage in nuclear waste materials can result in changes in volume, leach rate, stored energy, structure/microstructure, and mechanical properties [1]. As Matzke pointed out [2], a fundamental understanding of all interesting and important aspects of the interactions of radiation with the materials of interest and their possible effects on subsequent environmental degradation is still lacking. Questions deal with the essential changes in physical properties (e.g., volume), chemical properties (e.g., thermodynamic stability and leach rate), and stored energy as a function of radiation dose. It should also be pointed out that there is a priority to investigate the effects of electronic energy deposition on the physical properties [2].

How can the changes in physical and chemical properties be simulated in accelerated experiments to radiation dose of interest (waste form age of 10,000 years) is an area of interest [3]. Methods of studying the radiation damage in nuclear waste materials are [3]: (1) Actinide-doping, (2) Fast neutron irradiation, (3) Neutron induced reactions, (4) Fission-fragment damage, and (5) Charged particle irradiations [1]. Charged particle irradiations include electrons, protons, alpha particles, or heavy ions. They have the following advantages [1]: (1) Very short time, and (2) No difficulty associated with handling radioactive materials. However, they suffer from the following disadvantages [1]: (1) Correlation of damage produced by different particles is never straightforward, (2) Irradiation damage from a single particle type may be quite different from the real case, where the synergistic effects of all the radiation species are included. The following questions remain to be answered: (1) Surface damage vs. bulk damage, (2) Irradiation texturing of the surface, and (3) Small damage depth.

A number of naturally-occurring phases, including zircon ($ZrSiO_4$), pyrochlore ($A_{1-2}B_2O_6(O,OH,F)_{0-1}$), monazite ($CePO_4$), and uraninite ($UO_2$), are analogous to structure types that occur in ceramic and spent fuel nuclear waste forms [4]. These minerals (called metamict) can contain significant quantities of U and Th which, combined with their age (10^6 to 10^9 years), result in alpha-decay doses up to 10^{27} alpha-events/m^3 [4], (for these materials, a dose of 10^{15} alpha-events/mg is approximately equal to 10^{25} alpha-events/m^3 [5]). As a result, these minerals are found with a wide range of damage states ranging from highly crystalline to fully metamict (amorphous). A thorough understanding of radiation effects in natural minerals could help predict behavior in nuclear waste materials, as first suggested by Wing and Haaker [6].

RADIATION DAMAGE IN ZIRCON

Amorphization

Zircon can contain up to 0.6 wt. % UO_2 + ThO_2 and thus zircons, which are hundreds of millions of years old, experience doses up to 10^{16} alpha-events/mg (0.7 dpa) [4]. As early as 1864, zircon was the focus of study [7] and reviews of radiation damage in zircon are available [4,6]. It is one of the very few materials for which there are data that span a large range of relevant doses and times (up to 3×10^{16} alpha-decay/mg and 4×10^9 years) [8]. Zircon experiences a transition from the crystalline state (< 10^{13} alpha-decays/mg) to the amorphous state (>10^{16} alpha-decays/mg) [8]. When 2 MeV He ions were used to study radiation damage in zircon, an amorphous phase develops after an alpha dosage equivalent to some 10^{16} ions/cm^2. It is to be mentioned that most ionic oxides require the highest doses for amorphization (e.g., 10^{16} ions/cm^2 for quartz, or $5X10^{17}$ ions/cm^2 for sapphire). The amorphization dose for zircon is thus consistent with that expected for a primarily ionic bonding [9].

Mechanism of radiation damage

Alpha decay damage in minerals is the result of the decay of the naturally occurring radionuclides and their daughter products in the U^{238}, U^{235}, and Th^{232} decay series [4]. The damage is caused by two separate but simultaneous processes associated with the alpha-decay events: (1) An alpha particle (~4.5 MeV) with a range of 100,000 Å (i.e., 10 μ) dissipates most of its energy by ionization; however, at low velocities near the end of its track, it displaces several hundred atoms, creating frenkel defect pairs, and (2) The alpha-recoil atom (~0.09 MeV) with a range of 100 to 200 Å produces several thousand atomic displacements, creating "tracks" of disordered material [4].

Impact of alpha decay on zircon properties

It was noticed that fracture toughness of zircon increases and elastic moduli decrease with increasing alpha-decay dose [4]. Systematic pattern of microfractures perpendicular to the zones which contain variable amounts of uranium and thorium was observed. This is due to the differential expansion of the zones which experience alpha-decay doses in the range of 0.2 to 0.6 dpa. Also, the systematic pattern of microfractures provides rather dramatic evidence of changes in the mechanical properties of the material with increasing alpha-decay dose. There is also enhanced dissolution of zircon as a result of alpha-decay damage.

Alpha-decay induced amorphization and macroscopic swelling in natural zircons and actinide-doped zircon are similar, even though the dose rates differ by 10^8 [6]. Dose rates in natural zircon, and actual nuclear waste forms are < 10^3 and 10^4 to 10^9 Bq/g of alpha activity respectively [6]. Thus, there is no evidence for a significant dose-rate effects [6].

COMPUTER SIMULATION OF RADIATION DAMAGE IN ZIRCON

It was recently noted that accelerated simulation of changes in nuclear waste materials remains an essential question [3]. It was also noted that charged-particle irradiations is one of the techniques for simulating radiation damage in nuclear waste materials [1]. In the light of lack of funding for basic research in this area in the US and most other countries since about 1985 [10], computer simulation may offer an excellent source of information on radiation damage in nuclear waste materials. According to the author's knowledge; computer simulation for radiation damage in the waste materials was not considered before.

It should be mentioned that there is a need to properly estimate the partitioning of decay energy into electronic and nuclear energy losses to explain experimental results of the damage in zircon especially if we take into consideration that there is a priority to investigate the effects of electronic energy deposition on the physical properties [2]. Proper computer simulation offers such analysis.

Impact of compositional changes

Composition change in zircon may affect many parameters of interest in assessing radiation damage. One of the compositionally related parameters that may affect amorphization are weight percentage of SiO_2 and average atomic mass of a material. The latter is obtained by dividing the formula weight of the compound by the number of atoms in the formula [11]. Also, in the early stages of alpha decay damage, the density decrease is clearly dominated by contributions from the unit cell expansion. At higher alpha-decay doses, the change in density is most affected by the crystalline-to-amorphous transformation and perhaps by a continued decrease in the density of the aperiodic regions, as they are redamaged [12]. Thus, assessing compositional changes as a function of dose can be used to highlight mechanisms of this density change. The question also arises of the behavior of helium and oxygen atoms due to the atomic mixing and the resultant agglomeration of these gas atoms. Significant oxygen bubble formation was observed in ion irradiated waste glasses. This has been correlated to the ionization component of the energy deposition [13].

It is well known from the ion beam mixing techniques that at higher doses, changes in atomic mixing in the target should be taken into consideration and this would necessitate the use of dynamic simulation of the target. It is worth mentioning that ranges of the α-particle and the recoil atoms are very different: about 20 to 30 μm for the α-particle and about 0.025 μm for the recoil atoms in typical waste matrices [14]. Thus, if a specific phase of the waste matrix becomes enriched in actinides, this phase will encounter most of the atomic displacements since the recoil atoms will be stopped within this phase. However, since grain sizes in waste matrices and sizes of crystallites in glass ceramics are usually of the order of a few microns, the α-particle will effectively bombard and damage all of the waste matrix with its smaller damage rate and the more separated and dispersed displacements [14]. Thus, regardless of the fact that atomic mixing occurs at the end of the alpha tracks, each grain will suffer this kind of mixing.

What is really relevant here is to mention that recent work based on microcalorimetry, X-ray absorption spectroscopy and SIMS and electron microscopy has postulated the presence of zirconium- and silicon-rich domains which are less than 10 Å in size [15]. These domains have been identified at higher temperatures by neutron diffraction experiments [15].

Impact of high irradiation doses

There is a need for understanding the ability of a periodic structure to change as a function of increasing dose and in response to continuing alpha-decay damage [16]. High doses need to be studied when considering varying waste loading to be incorporated in zircon host matrix [17]. For a waste loading of 10 wt.% of Pu^{239} (half-life = 24,110 years), zircon will reach the saturation value of damage (1.2×10^{25} alpha-decay events/m^3 or 0.8 dpa) in approximately 1700 years [17]. It is thus obvious that there is a need to study levels of compositional changes in the transition dose between crystalline to metamict state. Then, this should be extended to higher doses.

Previous ion irradiations of zircon

Since it is unlikely that suites of natural specimens will provide samples for studying impact of varying alpha doses, we have to resort to ion implantation techniques to simulate the alpha-decay damage. Thus, a wider range of structure types (in various orientations) and compositions can be examined in materials simpler than natural systems and for which critical parameters (e.g., temperature) are controlled [16]. Most recently, particle irradiations have been used to induce amorphization in zircon, and the results were compared to the results of alpha-decay event damage [7]. This included (1) 2 MeV He, (2) 0.8 MeV Ne, (3) 1.5 MeV Ar, 1.5 MeV Kr, 0.7 MeV Kr up to 10^{15} ions/cm^2 [12], (4) 1.5 MeV Xe, and (5) Pb at 40-240 keV up to 10^{13} ions/cm^2, Pb at approximately 230 keV up to 10^{15} ions/cm^2, Pb at 14 MeV at 10^{11} ions/cm^2. All irradiations used singly charged ions.

Previous computer simulation for radiation damage in zircon

Ion range and damage profile calculations have been made using both the SUSPRE and TRIM codes [9] for 2 MeV helium ions for the dose of 8×10^{16} ions/cm^2. It was noted that depth scales derived from such computer codes are only accurate to about 15% and it was difficult [9] to directly decide the correlation between helium implant profile and damage to the investigated property changes due to alpha implantation.

TRIM code [18] was used to calculate 1.5 MeV Kr ion range in zircon. Because the electron transparent thickness is <0.3 μm and most ions penetrated this thickness, the chemical effect of implanted ions in the observed sample region is almost negligible [18].

Displacement damage and ionization energy profiles in zircon caused by 1.5 MeV Xe ions, 700 KeV Kr ions, 1.5 MeV Kr ions, and 400 KeV He ions were calculated [19] using TRIM code using displacement energy of 15 eV as well as 50 eV.

The average number of atomic displacements produced per alpha decay event from both the alpha particle and recoil nucleus was calculated with the Monte Carlo computer code TRIM-90 [20] assuming a displacement energy of 25 eV. Calculations were performed for both natural zircon and Pu-doped zircon.

Need for dynamic simulation of 4.5 MeV He ion irradiation on zircon

It is obvious that 4.5 MeV He ion irradiations were not carried before. Also, it is important to note that in previous simulations, only thin samples were used in the irradiations. This configuration does not allow the probing of the impact of nuclear atomic displacements and the subsequent atomic mixing on the compositional changes in zircon, especially at the end of the alpha track where nuclear energy deposition would dominate. Finally, as it is well known that computer simulation can offer quick and qualitative analysis for a wider ranges of experimental set ups even in cases where actual and exact parameters are nonexistent.

The use of a dynamic mode analysis is a main feature of the simulation which accounts for the change in composition of the target materials. This should be compared with the "static mode" in which target composition remains constant during irradiation simulation. This can be considered to be true for low ion fluences, typically under 10^{16} ions/cm^2. At high ion fluences, there should be a substantial modification of the target and the irradiating ions will be incorporated as one of the target species for the ions arriving later.

DYNAMIC MONTE CARLO SIMULATION OF RADIATION DAMAGE

The TAMIX code [21] was used for the Monte Carlo dynamic simulation. A moving atom loses its energy via nuclear and electronic stopping processes, which are independent on each other. Binary collision approximation is used for nuclear scattering between a moving atom and a target atom. The scattering angle is calculated using a repulsive screened Coulomb potential. For the mean free path calculations, the exponential distribution for the distance between successive collisions is used. Between nuclear collisions, a moving atom loses its energy continuously through electronic stopping process, which however, doesn't alter the direction of the moving atom.

The equation by Robinson [21] for the number of displaced atoms is used. Bragg formula [21] was used to determine the electronic stopping cross section of non-monatomic substances. For a target of molecules A_mB_n, the electronic stopping cross section is calculated from

$$S_e(A_mB_n) = m \times S_e(A) + n \times S_e(B) \qquad (1)$$

where $S_e(A)$ and $S_e(B)$ are the electronic stopping cross section of the target A and B respectively. The program uses electronic stopping power developed by Ziegler et al. [21], along with the velocity proportional formulae as in Lindhard's [21] for low energy region.

The dynamic simulation consists of first sectioning the target into different layers. After the termination of an ion history (including the specified number of the simulated secondary knock-ons), the net change in each layer is calculated. This new composition of the structure will enter into the simulation for the next set of PKA's and so forth.

Dynamic simulation of zircon (Zr + Si + 4 O atoms) was carried out for an initial atomic target composition of 15% for both zirconium and silicon, and 70% oxygen. A displacement energy of 25 eV was considered. The following ion irradiation experiments were simulated to investigate the spatial dependence of radiation damage and its associated electronic and nuclear energy loss: Ne (0.8 MeV), Ar (1.5 MeV), Kr (1.5 MeV), and Pb (230 KeV). Simulations were carried out for fluences of 10^{15} ions/cm^2. To reduce run time, only the PKAs (Primary Knock-on Atoms) were simulated for the Ar and Kr ions. The first SKA (Secondary Knock-on Atoms) were simulated in case of Pb ions. For the Ne ions, 4 SKA generations were also simulated.

Finally, and most important, an actual case of 4.5 MeV alpha particle was simulated to predict the radiation damage and the subsequent compositional changes in zircon due to the alpha decay. The following doses were considered: 10^{15}, 10^{18} and 10^{20} He ions/cm^2 representing different loadings of nuclear waste materials. To reduce run time, only the PKA and the first SKA were considered.

All simulations were carried out for semi-infinite media to properly account for the electronic and nuclear energy loss along the ion path. Simulations [18] for thin samples do not properly account for these variations as mentioned before.

Ion irradiations

Variation of electronic energy loss and nuclear energy loss per Angstrom for the different ion irradiations conditions are shown in Figures 1 and 2 as a function of depth of zircon. Different ratios of both electronic and nuclear energy losses for these ion irradiations are shown in Table 1.

Table 1 Electronic and nuclear energy losses of the different ion irradiations

Ion	Energy	% electronic energy loss	% Nuclear energy loss
$_{10}$Ne	800 KeV	17.3	82.7
$_{18}$Ar	1.5 MeV	25.5	74/5
$_{36}$Kr	1.5 MeV	60.2	39.8
$_{82}$Pb	230 KeV	90.9	9.1

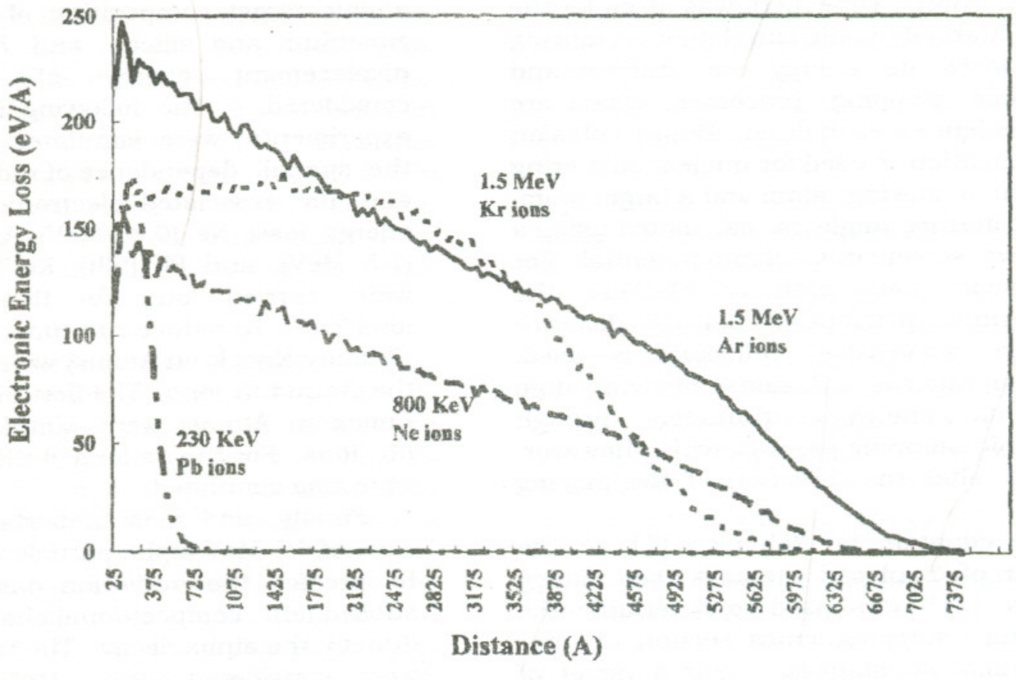

Figure 1 Electronic energy loss for 10^{15} ions/cm^2 incident on zircon

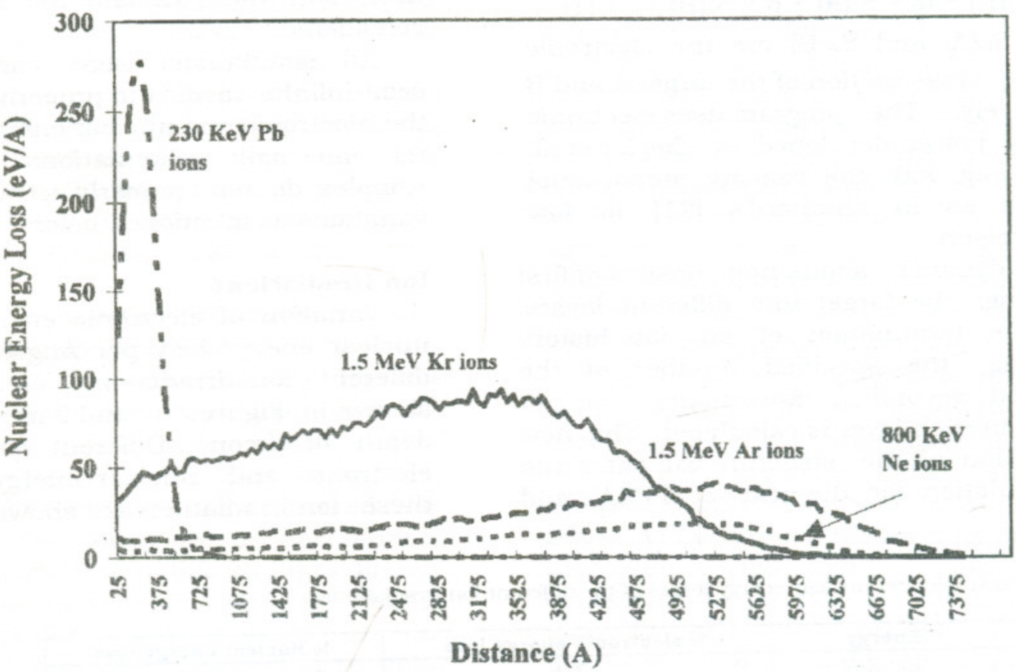

Figure 2 Nuclear energy loss for 10^{15} ions/cm^2 incident on zircon

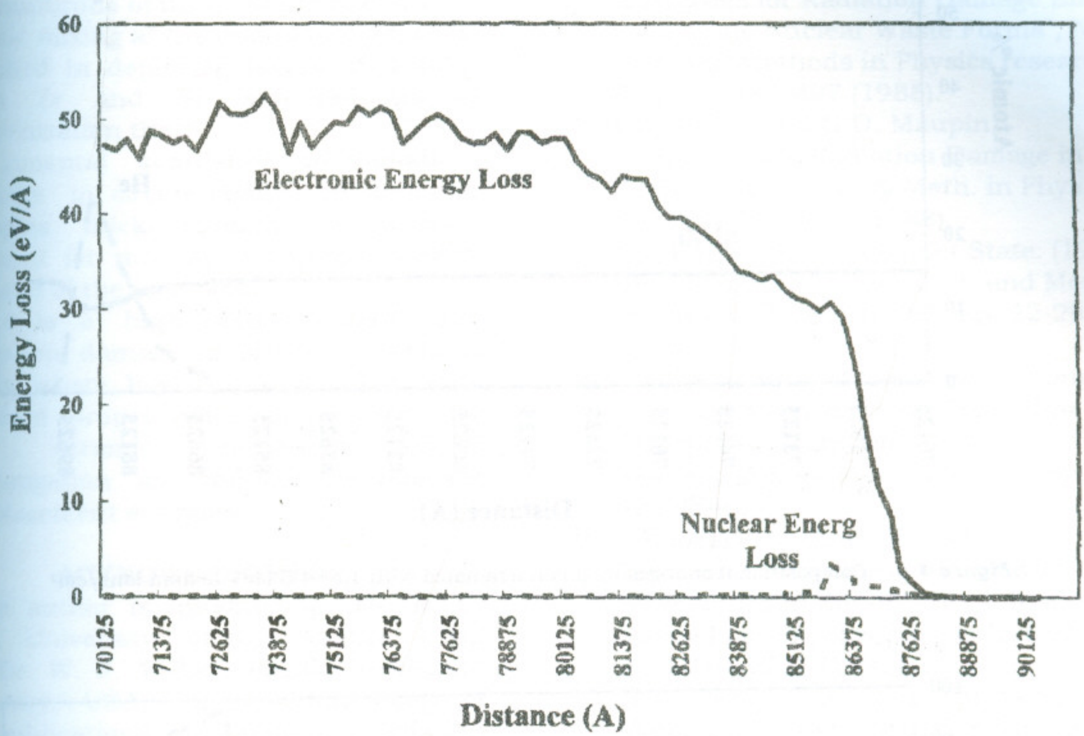

Figure 3 Electronic and nuclear energy loss for 10^{20} 4.5 MeV helium ions/cm² incident on zircon

From Figure 2, it is quite obvious that simulations for thin samples underestimate the nuclear energy loss especially for the Ar and Ne ions.

Helium irradiations

Electronic and nuclear energy loss as a function of depth in zircon samples are shown in Figure 3 for fluence of 10^{20} ion/cm^2. As expected the major mode of energy loss for the 4.5 MeV He ions is electronic energy loss, i.e., ionization effects (99.74%). However, by the end of the alpha track length, nuclear energy loss is noticeable.

Compositional changes at the end of the alpha track length are shown in Figures 4 and 5 for fluences of 10^{18} ion/cm^2 and 10^{20} ion/cm^2 respectively. All along its path length, compositional changes in Zr, Si, as well O were noticed. This is quite observable by the end of the alpha track, due to the concentration of nuclear energy loss mechanism there. Areas of about 1500 Å thick were totally depleted from Zr and Si. Also, the O atomic concentration there became appreciably small. Simulating small sample thickness would have missed such depletion layers. At a fluence of 10^{15} ion/cm^2 , target composition did not show the same noticeable variation.

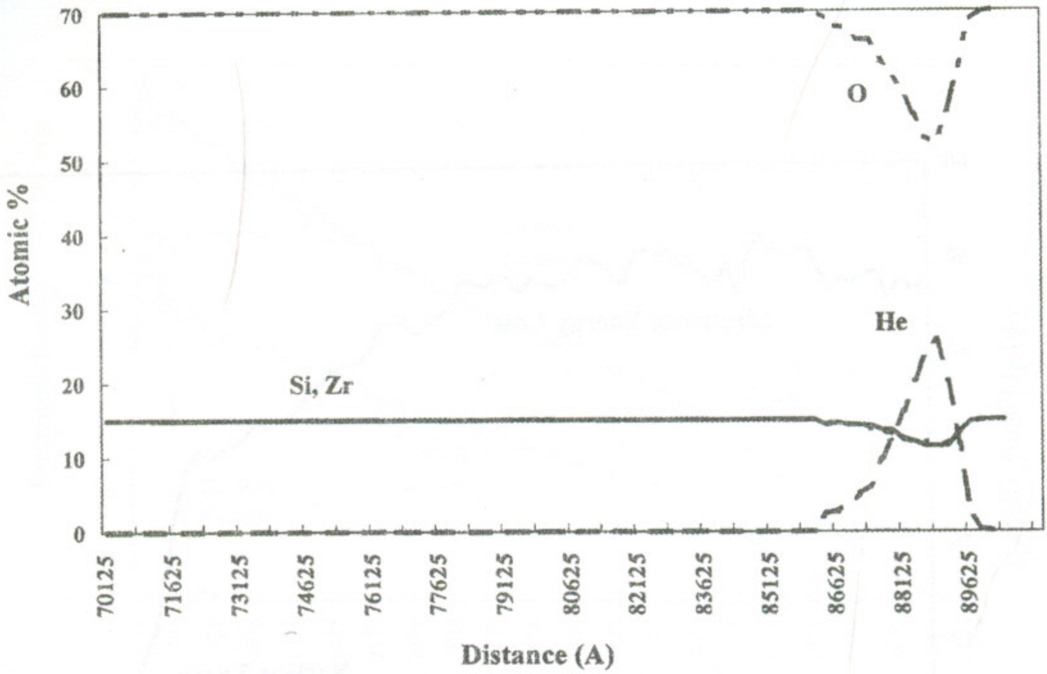

Figure 4 Compositional changes in zircon irradiated with 10^{18} 4.5 MeV helium ions/cm^2

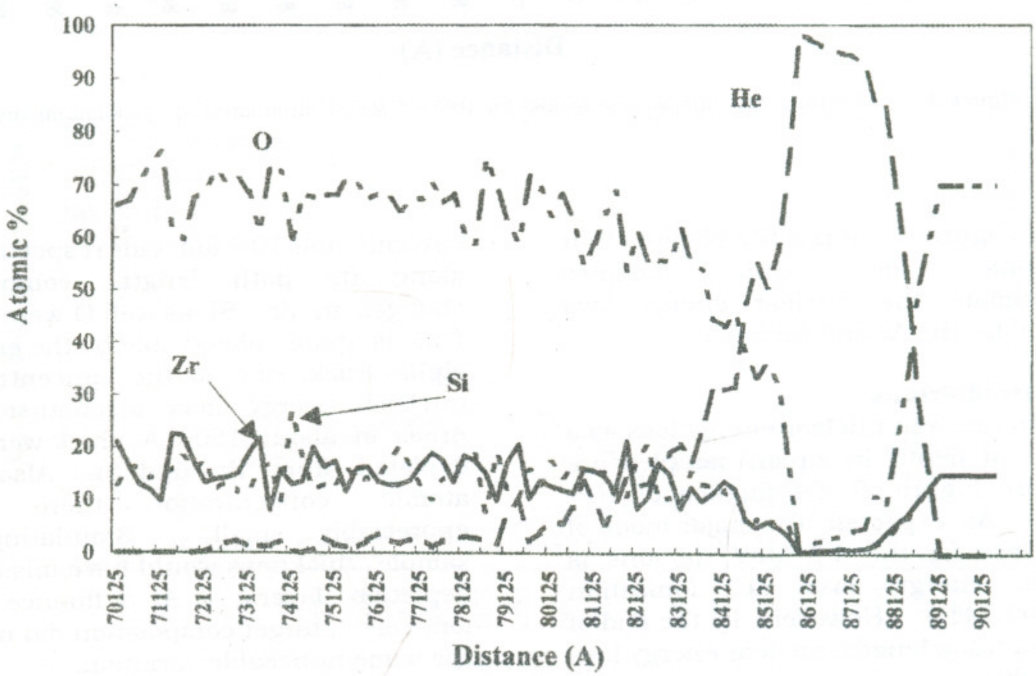

Figure 5 Compositional changes in zircon irradiated with 10^{20} 4.5 MeV helium ions/cm^2

CONCLUSIONS

1. Computer simulation of radiation damage in zircon offers a good opportunity for behavior analysis especially for different waste loading and the multitude of involved parameters.
2. Atomic mixing at the end of alpha tracks resulted in depleting layers of 1500 A from Zr and Si and reducing O concentration there.
3. Experimental simulation of radiation damage in zircon should be done for samples thick enough to properly account for nuclear stopping power by the end of the ion track.
4. There is a high need for simulating radiation damage in zircon as well as glass waste host matrices taking into account proper potential functions for the ceramic materials under investigation as well as the relevant displacement energies.

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المحاكاة الديناميكية للتلف الاشعاعى فى الزيركون نتيجة التحميل بالنفايات النووية

محمد حسن محمد
قسم الهندسه النوويه – جامعة الأسكندريه

ملخص البحث

تتعرض مادة الزيركون، والتى عادة مايبلغ عمرها عدة ملايين من السنين، الى تحول من الحالة البللورية الى الحالة العشوائية عند تعرضها لأشعة ألفا بكثافة مقدارها أكبر من ١٠^{٢٣} تحلل/م٣. هناك تكهنات بأن التغير فى مكونات الزيركون يكون له تأثير على تصرف مواد النفايات النووية الحاوى لها مثل ظهور انتفاخات موضعية فى تلك المواد. أثبتت التجارب الحديثة أن هناك مناطق فى الزيركون غنية بعنصر الزيركون وأخرى غنية بعنصر السليكون وذلك نتيجة لتعرضها للضرر الحادث من أشعة ألفا. تبلغ أبعاد تلك المناطق حوالى عشرة أنجستروم. مما هو جدير بالذكر أنه عند التعرض لجرعات عالية من الاشعاع لابد من الأخذ فى الاعتبار التغير فى التركيز الذرى للمواد المعرضة للتشعيع خلال فترة التعرض للاشعاع مما يتطلب اللجوء الى المحاكاة الديناميكية للمادة. وأخيرا، تجدر الاشارة الى ضرورة الدراسة الدقيقة لتأثير فقدان جسيمات التشعيع لطاقتها فى المادة نتيجة للتفاعل مع الكترونات المادة.

المحاكاة التى تمت فى السابق لتشعيع الزيركون بالأيونات كانت تتم لعينات ذات أسماك رفيعة وبالتالى لم تتم دراسة تأثير ازاحة الذرات من أماكنها فى المادة التى تمت محاكاة تشعيعها وكذلك الخلط الذرى الناتج وتأثيره على تركيب المادة خاصة فى نهاية مسار جسيمات التشعيع. فى الدراسة الحالية تمت محاكاة تأثير أيونات النيون (بطاقة ٠,٨ مليون الكترون فولت)، الأرجون (١,٥ مليون الكترون فولت)، الكريبتون (١,٥ مليون الكترون فولت)، وكذلك الرصاص (٢٣٠ كيلو الكترون فولت). تمت المحاكاة عند فيض أيونى مقداره ١٠^{١٥} جسيم/سم٢. كذلك تمت محاكاة تأثير جسيمات ألفا بطاقة ٤,٥ مليون الكترون فولت عند فيوض ١٠^{١٥} ، ١٠^{١٨} ، ١٠^{٢٠} جسيم/سم٢ والتى تمثل التشعيع نتيجة تحميل الزيركون بنسب متزايدة من النفايات النووية. فى كل أنواع المحاكاة السابقة، تم التمثيل الدقيق لفقد الأيونات لطاقتها نتيجة التفاعل مع الكترونات المادة وذلك فى عينات ذات أسماك أكبر من مدى الجسيم داخل المادة.