Master Nuclear Energy
Nuclear Reactor Physics & Engineering

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Nuclear Materials - Practical use of the SRIM computer-code program

I. Introduction

Some countries favour the direct disposal of spent nuclear fuels in geological repository in lieu of reprocessing, recycling uranium and plutonium and disposing fission products and unseparated actinides. The spent fuel is mainly composed of ^{238}U. This unstable uranium isotope, which is a (radioactive) actinide with a very long half-life (4.468×10^9 years), undergoes an alpha decay according to the following equation: $^{238}\mathrm{U} \rightarrow {}^{234}_{90}\mathrm{Th}(70\,\mathrm{keV}) + {}^{4}_{2}\alpha(4.2\,\mathrm{MeV})$; note that the ^{234}Th is unstable and rapidly becomes ^{234}U (after two β^- disintegrations that would induce a negligible damage).

1. For both types of particles, derive the initial ion velocity. Compare with the velocity of light. Comment.
2. Calculate the projectile velocity at the Bragg peak and infer the slowing-down regime of the penetrating ion.
3. Give an order of magnitude of the projected range of the two particles.
4. Define the lattice (E_{lat}) and surface (E_{surf}) binding energies. How the threshold displacement energy (E_d) differs from E_{lat}?
5. What is the minimum kinetic energy ($E_{K,min}$) of a Th projectile to create a permanent displacement of a U atom? And of an O atom? Considering that Th particles are in the range of 70 keV, comment the $E_{K,min}$ value.
6. What are the two phenomena that can lead to the damage of the UO_2 matrix during the alpha decay of actinides?

II. Use of SRIM

A. Description

SRIM, "Stopping and Range of Ions in Matter", is a program widely used in the field of ion irradiation. It calculates the stopping and range of ions into matter with a complete treatment of the ion-atom collisions. Calculations are performed in the frame of Monte-Carlo type simulations and within the binary collision approximation (BCA).

What is the main difference between the two principal simulation modes, "Quick" *vs.* "Full"?

B. Simulations

For the following simulations, the 'Calculation with full damage cascades' mode will be used. Let's assume that the corresponding actual experiments with an ion accelerator would be conducted with the same projectile/target couples up to a Th and He fluence of $\Phi=10^{16}$ cm^{-2}; note that this fluence would approximately correspond to the quantity of Th and He produced during ~0.7 billion years.

1. Perform a simulation of the interaction of 4.2 MeV He particles with a UO_2 target.
   a) Plot the "ionization" and "energy to recoils" depth profiles; what do they represent? Compare the results with those obtained in I.2.
   b) Plot the "ion ranges" distribution; what does it represent? Convert the unit of the ordinate axis into a more useful one. What is the value at the maximum of the distribution?
   c) Plot the "collision events" distribution; what does it represent? Convert the unit of the ordinate axis into a more useful one. Take note of the values at both the maximum of the distribution and at 10 nm.

2. Perform a simulation of the interaction of 70 keV ^{234}Th particles with a UO_2 target.
   a) Plot the "ionization" and "energy to recoils" profiles. Compare the results with those obtained in I.2.
   b) Plot the "collision events" distribution. Convert the unit of the ordinate axis into a more useful one, and take note of the value at the maximum of the distribution.
   c) Compare the values obtained at questions II.B.1.c and II.B.2.b. Comment.

III. Radiation damage induced by fission fragments

Fission fragments generated by the fission of ^{235}U and ^{239}Pu are the main source of radiation damage inflicted in urania during in-reactor operations. Using a similar approach as for the alpha decay, define your own SRIM simulations to simulate the slowing-down of a typical fission fragment in urania (e.g. Br, Kr, Zr as light fission fragments, and I, Xe, Ba as heavy fission fragments). The typical fission fragment fluence corresponding to a one-year irradiation time, $\Phi_{1y}=10^{17}$ cm^{-2}, allows you to estimate the number of displacement(s) per atom to which the UO_2 matrix fuel is submitted and then to compare such result with the radiation damage produced by alpha decay, i.e. both alpha and Th particles (be careful of the difference in the time of irradiation that is considered).

$\sqrt{\frac{2E}{m}} =$

<u>*Data and information:*</u>

UO_2: Molar mass, $M_{UO2} = (238.03+2\text{x}16.00) = 270.03$ g.mol^{-1};
Density, $\rho_{UO2} = 10.96$ g.cm^{-3}
E_d (U) = 40 eV; E_d (O) = 20 eV
$Z_U = 92$; $Z_O = 8$
Nucleon mass: $1.66\text{x}10^{-27}$ kg
Electron mass, $m_e = 9.1\text{x}10^{-31}$ kg
Avogadro number, $N_{av} = 6.023\text{x}10^{23}$ mol^{-1}
Bohr velocity, $v_B = 2.19\text{x}10^{6}$ m s^{-1}
1 eV $\leftrightarrow$ $1.6\text{x}10^{-19}$ J

Website address of the SRIM code: www.srim.org

<u>**Schematic evolution of electronic and atomic stopping powers versus ion velocity**</u>