22.01 Fall 2019, Problem Set 7

Complete all the assigned problems, and do make sure to show your intermediate work.

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1 (70 points) Skill Building Problems

1.1 (40 points) Radiation Damage in Metals

Learning Objective: These problems will help you understand radiation damage from the incoming particles to the end of defect creation. Understanding an individual radiation damage event is important for studying nuclear materials, since it is the accumulation of these events that leads to the property change of materials under irradiation.

Consider the case of a 3 MeV proton entering lead, and answer following questions with the help from the slides on the LMOD website.

1. (10 points) Describe what physical processes the proton may encounter as it enters into lead (how the proton loses its energy). Qualitatively draw the average energy of the protons versus the depth into lead. Which interaction mechanism is dominating at the beginning? At the end?

2. (3 points each)$\nu(T)$ is a parameter describing how many displacements a PKA (primary knock-on atom) with initial energy T produces on average. E_d is the displacement threshold energy, and is the minimum energy needed to displace a lattice atom. In class, you were given the Kinchin-Pease model as the following equation and graph. A few assumptions were made in describing this model. Now you are going to look more closely at those assumptions and see whether they are reasonable.

$$\nu(T) = \begin{cases} 0 & \text{for } T < E_{\mathrm{d}} \\ 1 & \text{for } E_{\mathrm{d}} \leq T < 2E_{\mathrm{d}} \\ \dfrac{T}{2E_{\mathrm{d}}} & \text{for } 2E_{\mathrm{d}} \leq T < E_{\mathrm{c}}. \\ \dfrac{E_{\mathrm{c}}}{2E_{\mathrm{d}}} & \text{for } T \geq E_{\mathrm{c}} \end{cases}$$

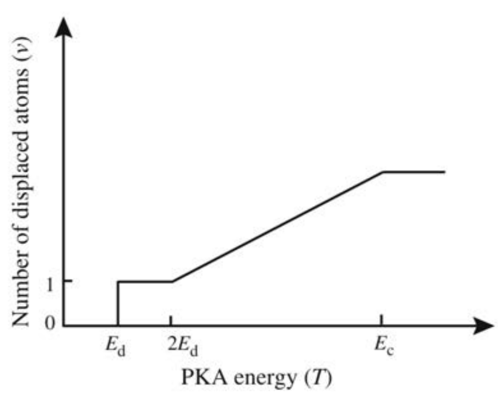

Figure 1: Kinchin-Pease model equation and graph.

(a) First assumption: "The cascade is created by a sequence of two-body elastic collisions between atoms." Is this always the case? Will $\nu(T)$ be bigger or smaller after relaxing this assumption?

(b) Second assumption: "The displacement probability is 1 for T bigger than E_d". Treating E_d as the threshold energy to cause one displacement, is this assumption true for room temperature and above? When will this be true?

(c) Third assumption: "When an atom with initial energy T emerges from a collision with energy T' and generates a new recoil with energy ε, it is assumed that no energy passes to the lattice and T = T' + ε". It is apparent that energy is not conserved in this assumption, what is the missing term? Will $\nu(T)$ be bigger or smaller after correcting this energy conservation?

(d) Fourth assumption: "Energy loss by electron stopping is given by a cutoff energy E_c. If the PKA energy is greater than E_c, no additional displacements occur until electron energy losses reduce the PKA energy to E_c. For all energies less than E_c, electronic stopping is ignored, and only atomic collisions occur." Is this true? What will happen when you correctly relax this assumption?

(e) Draw a suggested, updated curve for $\nu(T)$, relaxing the assumptions above. Label each change you make and just a 1-4 words describing each changed feature.

3. (15 points) We have learned that the displacements calculated using the K-P model are more than the actual point defects produced. To correct this, we simply multiplied the DPA equation with a correction term ξ, which is called "displacement efficiency." Researchers have put a lot of efforts to improve the accuracy of DPA calculation. Briefly go through this recent *Nature Communications* paper: https://www.nature.com/articles/s41467-018-03415-5. What have the authors presented as a correction of the NRT-dpa model? Briefly explain them and the advantages of them over the NRT-dpa model. (Can you sense what they are trying to do to make the damage calculation better at predicting or linking to macroscopic material property change?)

1.2 (30 points) Neutronics and Criticality

1.2.1 MIT Reactor Modifications (15 points)

Learning Objective: Intuitively discover what would happen to a nuclear reactor if certain changes were made during critical operation. Discover relationships between variables in the criticality relation.

For these questions, consider the MIT reactor in its critical state, and the various experiments that we do with it. >>>Here<<< is a cross section of the relevant parts of the MIT reactor. What would be the net effect of each of the following changes on the reactor's criticality, and **which of the terms in the one energy group criticality relation would be affected**? Explain why, using your knowledge of neutron absorption and leakage, and how they affect criticality.

(a) Passing silicon through the reactor to dope with phosphorus by transmutation ***(this really happens)***
(b) Throwing quarters directly in the core of the reactor like a wishing well ***(this actually happened!)***
(c) Closing all the beam ports which let neutrons out for experiments
(d) Raising the temperature of the coolant
(e) Increasing the enrichment of the fuel

1.2.2 Criticality Calculations (15 points)

Learning Objective: Actually calculate the physical size of critical reactor geometries, and find real cross section data on the JANIS database.

- (5 points) Using the one energy group criticality relation and cross section values taken at 2 MeV, calculate the radius of a perfectly critical sphere of ^{239}Pu surrounded by vacuum.

- (10 points) Develop a two energy group criticality relation *(fast (f) and thermal (th) energy groups)* in terms of only material properties & geometry, and use it to calculate the critical radius of a balloon filled with $^{235}UF_6$. Assume the $^{235}UF_6$ is stored at a density of $1\,\frac{kg}{m^3}$. You can simply pick average values in the fast (>1eV) and thermal (<1eV) energy regions, instead of doing any formal averaging.

– HINT: First check that an *infinite medium* would at least be critical, before accounting for the geometric buckling (physical size) of an enrichment plant.

2 Noodle Scratchers (30 points)

Will It Blend: AP-1000 Edition (30 points, answer not given)

Learning Objective: Perform true flux-averaged cross section calculations on a spreadsheet, and decide whether homogenizing a reactor which we know works would break it.

Read the >>>AP-1000 spec sheet<<< p. 7-9. Assuming that the core is completely homogeneous (blended) mix of fuel, cladding, coolant (assume $28.25\,\mathrm{m}^3$ at 303.4C), and structural materials (assume 5,920 kg), **calculate the criticality (k_{eff}) of the AP-1000 using homogeneous, two energy-group neutron diffusion theory** (two-group k_{eff} expression). What are the largest three factors which you believe make your k_{eff} not equal to unity? Be specific about what each would do to the two group criticality.

You may assume that the core contains only four materials: coolant/moderator (H_2O), fuel (UO_2), cladding $\underline{(assume\, pure\, {}^{90}Zr)}$, and structural materials $\underline{(assume\, pure\, {}^{56}Fe)}$. Ignore control rods, assume they are all out of the reactor during normal operation. Also ignore the reactor vessel or any other materials. You will have to calculate flux-averaged cross sections considering each isotope, for each energy group. ***Hints:*** You will have to take into account:

- Reactor operating temperature in Kelvin and density in $\left(\frac{g}{cm^3}\right)$ of the materials in the reactor
- Assume the fuel is 5% ^{235}U. Neglect any other isotopic abundances per the problem statement.
- Different diffusion coefficients for the two energy groups
- Perform your *microscopic* cross section averages using tabulated data from the ENDF/B-VII.1 cross section database for *incident neutrons*. Note that you can export the data directly, so you can perform the integrals in Excel or something similar, see the LMOD site for an example screenshot and an example spreadsheet. Discretize the energy integral using any method you see fit. You will have to compute flux-averaged microscopic cross section averages as follows: $\bar{\sigma} = \frac{\int \Phi(E)\sigma(E)dE}{\int \Phi(E)dE}$
  – ***Use the attached spreadsheet to obtain most of your values! I've done much of this work for you. You'll just have to export/obtain the values for U-235, and compute a couple of remaining values in yellow in the Final Calcs sheet.***
- Neglect photofission, (n, in) reactions, and anything else complicated
- Use the flux profile on the LMOD site (which contains a cross section averaging template) to compute your averaged macroscopic cross sections. Here is a plot of the flux spectrum: