SOTERIA COLLECTIVE EXERCISE

Session I: Irradiation damage and hardening for RPV.

How to launch the platform

- Open a terminal and go to the Perform folder
- Then, execute the following command “source env_perfect.sh” + click the SOTERIA logo on page 98 of the pdf presentation of the SOTERIA platform.

More details about the different modules used in this training session can be found in Ref. [1,2].

Exercise 1: Running the IRRAD+CONVOLVE chain

Once the PKA spectrum is obtained (through the IRRAD module), the final irradiation damage can be calculated through the use of a cascade database (for each temperature and PKA energy, cascade calculations are performed using Molecular Dynamics) and the CONVOLVE module. One can find in the folder /PDM/CONVOLVE/CASCADE different types of cascades (ANNEALED or RAW ones) for different classes of materials (pure iron or iron+Cu). One could obtain suitable information from the description of the different cascades, namely temperature, type of material and interatomic potential used for the Molecular Dynamics run.

Task 2-1: Restart the calculation and build a chain with the IRRAD and CONVOLVE modules with irradiation time (“time_irrad”) set to 1.303E+06 seconds.

Task 2-3: Run the chain

Question 2-3-2: Why is the “MD dpa” lower than the NRT dpa?

Task 2-4: Plot the vacancy and interstitial source terms. In order to do so, click on the Graphics tab, make the curve vSourceTerm and iSourceTerm visible and then hit the Apply button.

Task 2-5: Export the vSourceTerm and iSourceTerm as vSourceTerm.csv and iSourceTerm.csv. Then use the script as “gnuplot fit_source_term.gnu“ in order to obtain the exponent of a power law describing the source term of interstitials and vacancies. Are the exponents the same? Does it seem normal that there are more interstitial clusters (n>1) in the source term that vacancies? At this stage, should the equivalent number of mono-vacancies and interstitials be equal or not (example a di-interstitial as a contribution of 2 to the equivalent number of mono-interstitials)? Why ?

Exercise 2: Running the IRRAD+CONVOLVE+CRESCENDO+HARD chain

The chaining of IRRAD, CONVOLVE, CRESCENDO and HARD allows you to go from the neutron spectrum to the critically resolved shear stress (CRSS) increment and eventually the change in yield strength with the only knowledge of the neutron spectrum and some operating conditions (temperature and irradiation time). The rate theory model has been simplified to only include point defects generated during irradiation i.e. vacancies and interstitials: no solute atoms are explicitly included in such calculation even though this is in practice possible in AKMC for a full description of the chemical composition of RPV steel and in cluster dynamics for a one-solute model alloy.

Yet, a grey alloy approach (i.e. accounting implicitly for the presence of solute defects) can be tested in order to reproduce experimental data taken from PERFECT and PERFORM60 projects on model alloys (See figure 2 taken from reference [3]). The different samples have been irradiated in the test reactor BR2 at SCK-CEN up to a dose of 0.2 NRTdpa at a neutron flux of about 1.3×10^{-7} dpa.s^{-1} (corresponding to the SPECTER file br2-1.in.spe) and at a temperature of 573K. The goal of the exercise is to determine whether such a "grey alloy" approach is possible.

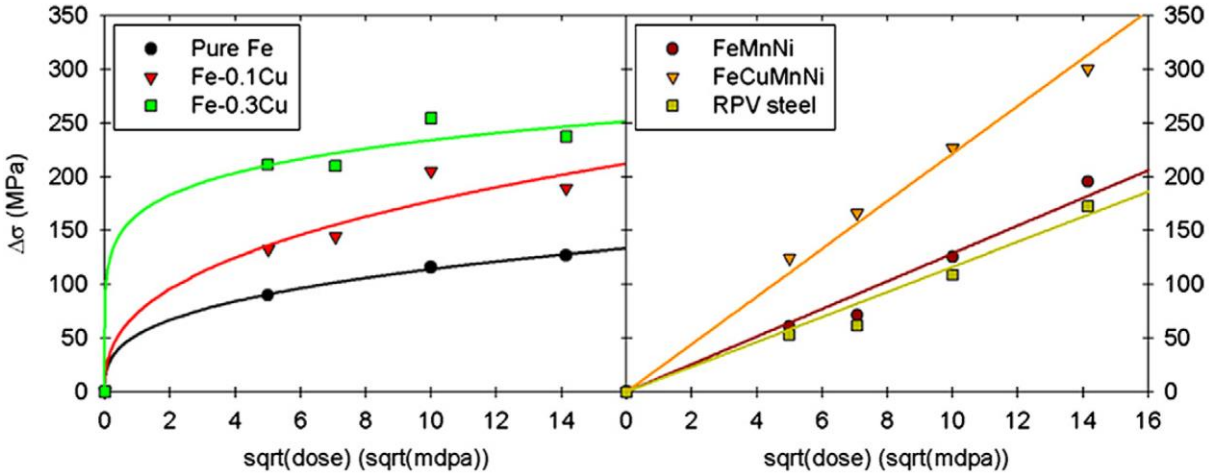

Figure 2: Variation of the yield strength for different model alloy and RPV steel as a function of the NRT dpa [3]

Task 3-1 Chain the module IRRAD, CONVOLVE, CRESCENDO and HARD. Then input the neutron spectrum file corresponding to BR2 high flux (br2-1.in.spe in the share/data/neutron_spectrum folder). Modify the time of irradiation to 1e6s. Run the chain. In the output section, click on the OUTPUT_DATA section and export the DeltaCRSSTable as a csv file named "DeltaCRSS.csv". This corresponds to the variation of the critically resolved shear stress (CRSS) corresponding to the appearance of a population of voids and dislocation loops originating from the evolution of the primary damage. The variations of CRSS are directly related to the variation of the uniaxial yield strength through the Taylor factor (2.5-3.06 for RPV steel). Use the gnuplot script provided with the collective exercise ("gnuplot fit_delta_crss.gnu") to compare the data generated with the experimental ones. Be careful, the yield strength variation is plotted versus the NRT dpa as it is usually done in the academic literature. What do you observe ?

Microstructure changes under irradiation

The previous task clearly shows that macroscopic quantities are insufficient to clearly describe the microstructure evolution under irradiation. Considering Small Angle Neutron Scattering data taken from [4], on pure iron under the same irradiation conditions, one can evaluate the distribution of voids in the material and compare it with the result of the microstructural modelling.

Task 3-2: Switch to the expert mode in the User profile, then look for the OUTPUT_DATA for irradiated_microstructure/vacancies_final_volume_fraction_per_radius/table_for_optimisation, click on the plot button and compare the results with the solid line in the figure 3. Is the concentration of voids under or overestimated?

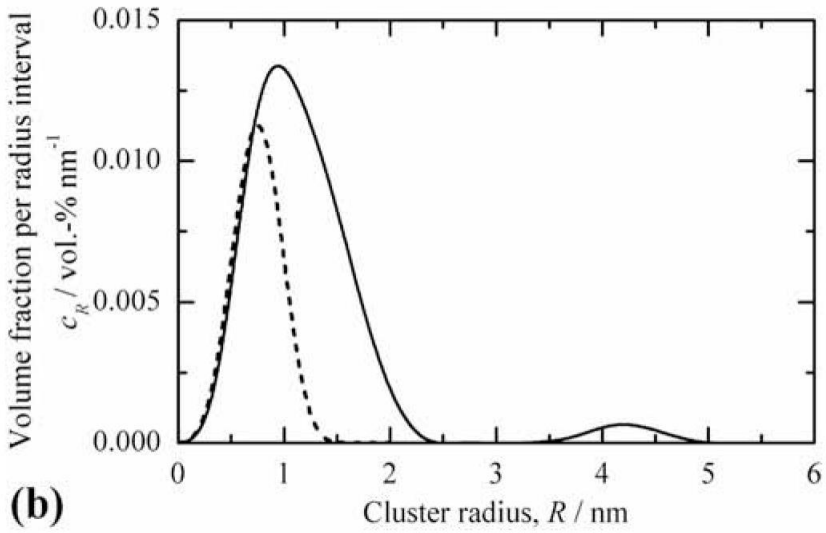

Figure 3: Distribution of vacancy clusters in pure iron for 0.19 dpa (plain line) and 0.038 dpa (broken line)[4]

Task 3-3: You can also obtain the average size and average concentration of the interstitial loop populations and compare it to the experimental data from PERFECT project (TEM data [5]): average mean radius is 5-8 nm and average concentration between $5x10^{15}$ and 10^{16} cm^{-3} for pure iron and 0.19 dpa. Is the simulated microstructure in good agreement with experiments?

Effect of carbon

If we want to compare the simulated cluster distributions with experimental ones, we have to take into account some of the important experimental constraints. It is very difficult to synthesize ultra-pure iron, for example carbon pollution is very likely to occur typically at 10 ppm level. Carbon acts as a very efficient trap for mono-vacancies, it can form complexes which trap the vacancy until the "bond" is broken. Ab initio calculations yields the following values for vacancy-carbon interactions:

- V_1 migration energy in pure α-iron about 0.67 eV

- V_1C_1 binding energy about 0.44 eV
- V_1C_2 binding energy about 1.5 eV

Task 3-4: Let us treat the mono-vacancy migration energy as an effective parameter accounting for migration of the vacancy after the dissociation of the carbon-vacancy complexes ("grey" alloy parameterization) we can safely adjust this parameter between 0.67 and 1.5 eV. Which value of the migration energy of the mono-vacancy fits best the experimental yield strength variations? Is it coherent with the binding energy values obtained from ab initio calculations? What is the effect on the decreased diffusion coefficient on the distribution of voids? on the average radius of interstitial loops ?

Towards a grey alloy model for Fe-Cu model alloy

You can load the study Fe-pure.prf where some parameters of the cluster dynamics have been modified so as to reproduce experimental results namely:

- The void distribution at 0.2 dpa [3]
- The average mean radius and concentration of interstitial loops at 0.2 dpa [5]
- The CRSS at 0.2 dpa.[3]

Some constraints have been imposed to: source term is taken from the CONVOLVE module without any modifications, $Z_i > Z_v$, 0.7 eV $< E_m$(mono-vacancy)$<$ 1.3 eV.

Task 3-5 Verify that the model reproduces the experimental data, does it describe satisfactorily the evolution of CRSS as a function of dpa?

Task 3-6 Considering that addition of Cu in the alloy will (i) induce the formation of mixed Cu-V clusters with higher mobility than the pure vacancy clusters due to the 0.2 eV binding energy between Cu and V and (ii) decrease the mobility of interstitial loops due to the 0.2-0.3 eV binding energy between Cu and <110>-dumbbell or <111> dislocation loops. Which parameters have to be modified to account for such behaviour? Modify the parameters accordingly (load the study fecu_crescendo.prf): the number of mobile species for vacancy-based clusters has been increased (m_v ↗), the migration energies of vacancy and interstitials have been increased to account for the trapping effect of Cu. How does the volume fraction of voids evolve with respect to the case of pure iron (See figure 4)? Concerning the interstitials loop, does the value at 0.2 dpa agree with the experimental value (average mean radius 2-3 nm and 10^{15}-$5x10^{15}$ cm^{-3}) ? Check the evolution of the CRSS with respect to the dpa: do you find a good agreement ? What is the likely missing ingredient in the cluster dynamics model?

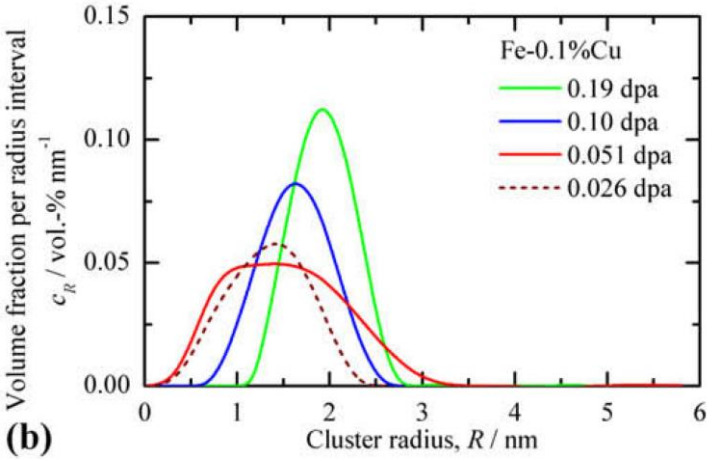

Figure 4: Distribution of vacancy clusters in model alloy Fe-0.1Cuat% for different fluences.[3]

[1] G. Adjanor, et al., Journal of Nuclear Materials, 406, 175 (2010)

[2] S. Bugat et al., Journal of Nuclear Materials, 406, 166 (2010)

[3] M. Lambrecht et al., Journal of Nuclear Materials, 406, 84 (2010)

[4] F. Bergner et al., Journal of Nuclear Materials, 399, 129 (2010)

[5] M. Hernandez Mayoral. PERFECT Project , Deliverable P26, Task II-3-2, 2005.