REQUIREMENTS FOR THE DUAL Fe + H/He BEAM AT THE ACCELERATOR HIPR FOR SIMULATION OF NEUTRON INFLUENCE ON NUCLEAR REACTOR MATERIALS

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Abstract. Ion accelerator facility is a powerful tool that can be used to simulate neutron irradiation effects in reactor materials. At the NRC “Kurchatov Institute” - ITEP the heavy-ion accelerator HIPr is used for the ion-beam simulation of radiation damage in steels and alloys. Irradiation is provided with the wide range of metal ions (mainly Fe²⁺). It is essential to include helium and hydrogen beams for the proper simulation of transmutation driven mechanisms of swelling and void formation. Energies, beam line angle and intensity are determined for design of the second beam line for He/H implantation at HIPr.

1. Introduction

Development of structural materials for new generation of advanced fission and fusion reactors requires the understanding of material properties and microstructure changes due to neutron irradiation [1]. Ion beams are used to simulate neutron radiation effects on nuclear reactor materials [2]. Ion irradiation can produce the most of microstructural changes observed in neutron irradiated materials (dislocation loops, cavities, solute segregations, precipitates, etc.). The ion irradiation experiments have benefits of low material activation and controlled variation of irradiation conditions such as temperature, dose rate, fluence, etc.

Since 2009 Heavy Ion Prototype (HIPr) facility located at NRC "Kurchatov Institute" – ITEP (ITEP) is used for simulation of radiation effects in promising reactor structural steels and alloys by irradiation with accelerated heavy ions (Fe, Ti, V et al) of [3]]. The HIPr is a RFQ linear accelerator operating with an ion beam pulse duration of 450 µs and a repetition rate one pulse per two seconds. The ion beam is accelerated up to total energy of 101 keV per nucleon (5.6 MeV for iron). The irradiated specimen size is Ø 3 mm and thickness of 0.1 mm. During irradiation the specimens are kept under fixed temperature (in the range from room temperature up to 500°C).

The heavy ions irradiation experiments simulate only defect production in a material. Helium and hydrogen implantation can be used to simulate transmutation effects in heavy ion damaged area [7]. In
the work [8], it is shown that dual and triple ion beams irradiation facilities are required to investigate
the synergistic behavior of gas accumulation and radiation defect generation in reactor materials. Around
the world, a several dual and triple ion beam facilities are already involved into simulation studies of
material radiation resistance. They are TIARA [9], DuET [10], HIT [11], FZ Rossendorf [12], FSU Iona
[13], LANL [14], JANNUS [15]-[16], the facility at Oak Ridge National Laboratory [17], the facility at
Michigan Ion Beam Laboratory [18] and some facilities at Kharkov Institute of Physics and Technology
[19][21].

At HIPr it is planned to build the second beam line for the implantation of H or He ions in specimen
simultaneously with heavy ions irradiation. Parameters of hydrogen or helium beams required to keep
fixed ratio between generated defects and implanted gas ions along investigated area of the sample are
presented.

2. Calculation with the SRIM code
To determine the damage profile in irradiated specimens, SRIM (Stopping and Range of Ions in
Materials) code was used [7]. The modeling of Fe ion implantation and energy losses was carried out
according to the procedure described in [23]. For modeling the SRIM mode “Ion Distribution and Quick
Calculation of Damage” was used with following parameters: (i) Fe ion beam with the energy of
5.6 MeV irradiating the 100% iron specimen under 90° angle to specimen surface; (ii) displacement
threshold energy is 40 eV; (iii) lattice binding energy is 0 eV. According to [23] for damages $N_d(x)$ [dpa]
calculation the formula was used:

$$N_d(x) = 0.8 \cdot \frac{f_{Fe}}{n_{Fe}} \cdot \frac{E^p(x) + E^P(x)}{2E_d} \cdot 10^8,$$  (1)

where $f_{Fe}$ is the fluence of Fe ion beam [cm$^{-2}$], $n_{Fe}$=8.48·10$^{23}$ cm$^{-3}$ is the specimen number
density (Fe 100%), $E_d$=40 eV is the displacement energy, $E^p(x)$ is the distribution of beam energy
lost to phonons (the SRIM result), $E^P(x)$ is the distribution of target atom energy lost to phonons
(the SRIM result), 10$^8$ is a multiplier scaling Å to cm. Solid lines in Figure 1 show the damage profile
(blue) and implanted ion profile (red) in iron specimen if the beam is perpendicular to the specimen
surface.

The investigation range of the defects generated by ion beam has upper and lower depth limits. The
lower depth limit is defined by the requirement to exclude the surface effects. Near the surface, a
depleted defect zone is typically observed in irradiated materials. The upper limit is defined by the
requirement to exclude the too high concentration of the implanted ions. The implanting ions may exert
excess-interstitial defect imbalance effects. An increase in the temperature of the sample leads to an
increase in the influence of the interstitial and surface effects. Therefore, investigation range of the
defects decreases with temperature increase. In work [24] analysis of the ion irradiation depth profile
was provided for iron samples irradiated by 5 MeV Fe ion beam. The differences in implantation of Fe
5.6 MeV and 5 MeV ions (fig. 1 dash-dotted line) are not significant in depth; therefore, we used results
from [24] to define the upper and lower depth limits. For example, lower depth limit is 300 nm for
irradiation of samples with room temperature (minimal) and every dpa. The upper depth limit is 650 nm
for irradiations up to 100 dpa under 550°C (the same as for irradiation up to 200 dpa under 500°C).
Therefore, the depth range from 300 nm to 650 nm was chosen for following modeling.

He and H implantation depth dependence on energies and angles to specimen surface was
investigated in [25]. According to the results, the angles with more than 15° critically reduce
implantation depth. From other hand the small angle of gas ion beam causes difficulties of target tank
construction if the ion beam falls on target perpendicularly to the specimen surface.

If the specimen surface is rotated 15° to Fe ion beam axis, the Bragg’s peak depth of implanted Fe
ions is moved from 1400 nm to 1350 nm (see Fig. 1 dashed lines). As result the angle of 30 degrees
between the iron and He/H beam lines with target surface rotated 15° to both ions axes was chosen for
the second beam line (see Fig. 2). All modeling results presented below were obtained for this geometry.
Figure 1. Damage and ion implantation profiles in the iron sample irradiated with Fe ion beam to the fluence of $10^{16}$ cm$^{-2}$ with 0° and 15° angle to the specimen perpendicular.

Figure 2. Layout of design dual beam

As it was mentioned above the main goal of the work is to define the modes of gas implantation (both hydrogen and helium) providing the constant ratio between implanted gas ions and number of defects generated by Fe ion beam along the specimen depth range acceptable for simulated radiation condition. The profile of He and H implanted in the specimen by ion beam has a peak width thinner than the defined upper range from 300 nm to 650 nm. Therefore to provide required distribution of implanted gas ions the implantation with different beam energies $W_i$ and fluencies has to be carried out. The distribution of implanted gas ions ($n_{gas}$) is defined as a production of beam fluence $f_l_i$ and distribution $dist(x,W_i)$ defined by the SRIM calculation. Below the index "gas" is used for general case of He and H ions/particles and indexes “He” and “H” when the specific ions is discussed:

$$n_{gas}(x,W_i) = f_l_{gas} \cdot dist(x,W_i).$$

(2)

Summed distribution of gas ions implanted with different energy $W_i$,defines as:

$$n_{gas}(x) = \sum_i f_l_i \cdot dist(x,W_i).$$

(3)
It is comfortable to use the total gas ion beam fluence \( f_{l_{\Sigma}} = \sum f_{l_i} \) and introduce the fraction coefficient \( k_i \):

\[
n_{gas}(x) = f_{l_{\Sigma}} \sum k_i \ \text{dist}(x, W_i),
\]

(4)

where

\[
k_i = \frac{f_{l_i}}{f_{l_{\Sigma}}}
\]

(5)

The distributions of implanted gas ions for set of beam energies \( W_i \) were obtained by SRIM. Using these distributions, to provide the summed distribution of implanted gas ions similar to the distribution of defects generated by iron ion beam in specimens, fluence fractions \( k_i \) for all energies \( W_i \) were determined.

First, the set of \( k_i \) coefficients was obtained for He ion beam implantation. For helium implantation into iron in depth of 300 nm and 650 nm depth, the beam energy \( W_i \) is 100 keV and 300 keV respectively. The implanted ion profiles \( \text{dist}_{He}(x, W_i) \) were obtained by varying \( W_i \) with 50 keV step. Coefficients \( k_i \) were fitted to obtain the summed profile \( \text{dist}_{He}(x, W_i) \) with similar to damage profile generated by Fe ion beam with 5.6 MeV. Figure 3 illustrates the modelling results of \( n_{i He}(x, W_i) \) for energies \( W_i \) of 100 keV, 150 keV, 200 keV, 250 keV, and 300 keV, summed profile \( n_{\Sigma He}(x) \) and profile of damages \( N_d(x) \) generated by Fe ion beam. The ordinate axis has arbitrary units for comparing shapes \( n_{\Sigma He}(x) \) and \( N_d(x) \) only. The shapes of summed profile \( n_{\Sigma He}(x) \) and profile of damages \( N_d(x) \) are similar in the range from 300 nm to 650 nm. Table 1 presents the set of coefficients \( k_i \) that was used for \( n_{\Sigma He}(x) \).

![Figure 3. Profile of damages, profiles of He implantation with different energies and its sum.](image)

### Table 1. Coefficients for He implantation

| He ions energy \( W_i \), keV | 100  | 150  | 200  | 250  | 300  |
|------------------------------|------|------|------|------|------|
| \( k_i \)                    | 0.15 | 0.19 | 0.12 | 0.15 | 0.39 |

The hydrogen implantation modelling was made the same way as the helium one. To implant hydrogen ions into iron in depth of 300 nm and 650 nm, the beam energy \( W_i \) is 50 keV and 150 keV respectively. The implanted ion profiles for different beam energies \( \text{dist}_{H}(x, W_i) \) were obtained by...
varying $W_i$ with 25 keV step. However, using such step it is impossible to determine the set of coefficients $k_i$ needed to obtain the required sum profile $n_{EH}(x)$. Therefore the additional profile $dist_H(x, W_i)$ for hydrogen ion energy $W_i$ of 60 keV was defined and used for modelling $n_{EH}(x)$. Figure 4 shows the results of SRIM calculation of $n_H(x, W_i)$ for the energy $W_i$ of 50 keV, 60 keV, 75 keV, 100 keV, 125 keV, and 150 keV, sum profile $n_{EH}(x)$ for hydrogen ion beam implanted in iron and profile of damage $N_d(x)$ generated by Fe ion beam in the same specimen. Table 2 has set of coefficients $k_i$ that was used for $n_{EH}(x)$.

According the obtained results, to provide the required profile of implanted helium or/and hydrogen ions in studied iron specimen at a depth from 300 nm to 650 nm, a ~300 kV electrostatic field can be used to accelerate $\text{He}^+$ and $\text{H}^+$ ion beams.

![Figure 4](image)

**Figure 4.** Profile of damages, profiles of H implantation with different energies and its sum.

| H ions energy $W_i$, keV | 50  | 60  | 75  | 100 | 125 | 150 |
|--------------------------|-----|-----|-----|-----|-----|-----|
| $k_i$                    | 0.1 | 0.09| 0.12| 0.18| 0.17| 0.34|

### 3. Calculation of He / H fluence

To design the gas beam line, it is necessary to define the currents of He and H ion beams required for the experiment. Let’s first determine helium and hydrogen fluences required. To determine the required fluences, the value $aim$ characterizing the ratio of depth distribution for gas accumulation in material $\rho_{gas}(x)$ [atomic particle per million] to damage profile $N_d(x)$ [dpa] is used:

$$aim = \frac{\rho_{gas}(x)}{damages(x)}$$

$$\rho_{gas}(x) = \frac{n_{gas}(x)}{n_{Fe}} \cdot 10^6.$$  

The equation (7) is used for 300 nm $< x < 650$ nm. Using equations (1), (4), (6), (7) one has:
The ratios of gas ion beam fluence to Fe ion beam one required for fission, fusion and spallation facilities can be taken from Error! Reference source not found.. Therefore, to define the He or H ion beam currents required for experiments, equation (8) with the results presented in Fig. 3 & 4 and tables 1 & 2 can be used. At HIPr the Fe\(^{3+}\) beam current is equal to 220 μA on the specimen surface (irradiated area is 9.6 mm\(^2\)). The required He\(^{+}\) and H\(^+\) beam currents (\(I_{He}\) and \(I_H\)) were determined for the same pulse duration and the repetition rate as Fe\(^{3+}\) beam. The result is shown in table 3. The H\(^+\) beam current \(I_H\) varies from 0.0165 μA to 3.3 μA to simulate features of materials for different facilities (table 3). The H\(^+\) beam current \(I_H\) varies from 7.15 μA to 160 μA.

| Facilities          | \(\text{aim}_{He}^{[\text{dpa}]}\) | \(\frac{fI_{He}}{fI_{Fe}}\) | \(I_{He}\) [μA] | \(\text{aim}_{H}^{[\text{dpa}]}\) | \(\frac{fI_{H}}{fI_{Fe}}\) | \(I_{H}\) [μA] |
|---------------------|-------------------------------|-----------------------------|-----------------|-------------------------------|-----------------------------|-----------------|
| Fission (Gen I)     | 0.1                           | \(1.5\cdot10^{-4}\)         | \(1.65\cdot10^{-2}\) | -                             | -                           | -               |
| Fission (Gen IV)    | 0.2                           | \(3\cdot10^{-4}\)           | \(3.3\cdot10^{-2}\) | -                             | -                           | -               |
| Spallation (DEMO)   | 10                            | \(1.5\cdot10^{-2}\)         | \(1.65\)        | 45                            | \(6.5\cdot10^{-2}\)         | \(7.15\)        |
| (full power year)   | 200                           | \(0.3\)                     | \(3.3\)         | 1000                          | \(1.45\)                    | \(160\)         |

4. Summary

To design the second beam line at the HIPr facility for ion beam simulation experiments, the 15 degrees angle between the gas beam line and the specimen surface normal was chosen. The same angle between iron beam and specimen surface normal was chosen as well. Therefore, the angle between two beam lines is 60 degrees. The helium beam energy variation in the range from 100 keV to 300 keV as well as the hydrogen beam energy variation from 50 keV to 150 kV is required for the experiments. The beam currents for helium and hydrogen ion beams required to simulate the different fusion and fission reactor conditions were determined. These results will be used to design the second beam line at HIPr.

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