Simulation of Fe-Ion Irradiation Damage in the MSR Structural Material Hastelloy N under KAHIF Irradiation Conditions Using SRIM

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1. Introduction

Molten salt reactors (MSRs) operate in high-temperature molten salt environments, and the corrosion resistance of structural materials is critical for reliable long-term operation. Hastelloy N is a representative candidate alloy for MSR systems owing to its favorable high-temperature properties and corrosion resistance in molten salt environments [1]. Under MSR operation conditions, structural materials are exposed not only to corrosive molten salts but also to neutron irradiation, and irradiation-induced defects can alter microstructure and transport pathways, which may influence subsequent environmental response [2]. Direct neutron irradiation experiments are costly, time-consuming, and constrained by facility availability, therefore heavy-ion irradiation offers an accessible and controllable approach for introducing irradiation damage in laboratory studies [3]. Heavy-ion irradiation typically yields a near-surface, depth-dependent damage profile with implantation effects, so the damage level and depth distribution should be quantified. In this context, quantifying the damage level and its depth distribution provides a practical basis for designing and comparing ion-irradiation conditions. In this work, Fe ion irradiation is employed as a representative heavy-ion condition for Hastelloy N. Depth-dependent displacement damage and Fe implantation profiles are estimated using the SRIM simulation code to describe the resulting irradiation damage state [4].

2. Irradiation conditions and SRIM calculations

2.1. Irradiation parameters at KAHIF (RFQ-based)

The heavy-ion irradiation parameters employed in this work are defined within the operational limits of the Korea Atomic Energy Research Institute Heavy Ion Irradiation Facility (KAHIF). At KAHIF, heavy ions are accelerated using a radio-frequency quadrupole (RFQ), which provides a fixed beam energy of 172 keV per nucleon. Under this RFQ-based configuration, the total ion energy is determined by the mass number of the ion species; for Fe ions in the 13+ charge state, this corresponds to a beam energy of approximately 9.63 MeV. In addition to ion energy, the beam current, irradiated area, and irradiation time are parameters required to define fluence. In the present work, these quantities are treated as assumed reference values for damage calculations rather than as experimentally realized irradiation conditions. The irradiation parameters adopted for the calculations are summarized in Table 1.

Table. 1. Parameters adopted for SRIM calculations at KAHIF.

Ion species	Charge state	Beam Energy	Beam Current	Area (Assumed)	Time (Assumed)
Fe	13+	9.632 MeV	1 μA	1 cm^2	1 hr

2.2. Material input parameters for SRIM calculations

For SRIM-based displacement damage calculations, material-specific inputs were defined in addition to the irradiation conditions, including the elemental composition of Hastelloy N and the displacement energy assigned to each constituent element. Hastelloy N was treated as a multi-component alloy with nominal weight fractions, and element-specific displacement energies were adopted from commonly used literature values, which are summarized in Table 2.

Table. 2. Chemical composition of Hastelloy N and displacement energies used for SRIM calculations.

Element	Wt. %	E_d (eV)
Ni	Bal.	40
Fe	4.28	40
Cr	7.25	40
Mo	16.56	60
C	0.06	28
Mn	0.48	40
Si	0.27	15
P	0.005	25
S	0.002	25
W	0.1	90
Co	0.1	40
Cu	0.1	40
B	0.003	25

2.3. Calculated damage and implantation profiles result

Depth-dependent displacement damage and Fe ion implantation profiles were calculated using the SRIM code under the defined irradiation conditions. Figure 1(a) shows the resulting dpa and Fe concentration profiles as a function of depth. The damage profile exhibits a subsurface maximum at ~1.8 μm, whereas the implanted Fe concentration is confined to a narrower region and peaks slightly deeper at ~2.05 μm. These profiles quantify the spatial distributions of displacement damage and implanted ions. Figure 1(b) presents a five-level irradiation damage matrix defined by fluence control, corresponding to peak damage levels of 1, 2, 5, 10, and 20 dpa. The fluence for each target peak dpa was obtained by linear scaling using the SRIM-derived damage yield per unit fluence. This stepwise matrix enables quantitative definition of near-surface damage across irradiation levels and allows extraction of an effective damage zone (from the surface) based on a selected dpa reference level, providing a practical metric for subsequent molten-salt corrosion study design.

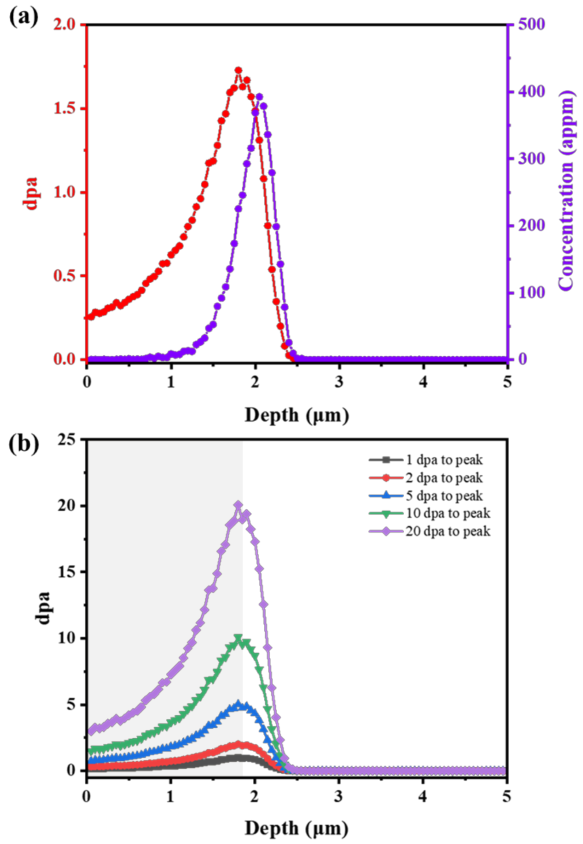

Figure. 1. (a) SRIM-calculated dpa and Fe ion concentration profiles n Hastelloy N. (b) Stepwise dpa profiles defined by fluence scaling.

In addition to the RFQ-based conditions, a higher-energy scenario was considered by assuming further acceleration using an interdigital H-mode (IH) structure at KAHIF. This configuration provides an incident energy of 1.06 MeV/u, corresponding to ~59 MeV for Fe ions, and the SRIM-calculated displacement damage and Fe implantation profiles are shown in Figure 3. The higher ion energy shifts both the damage peak and implanted-ion distribution to greater depths; the damage maximum occurs at ~5.2 μm and the Fe concentration peaks slightly deeper at ~5.4 μm. This higher-energy case expands the accessible damage-depth range, enabling the irradiation-damaged region to be positioned deeper when defining conditions for subsequent molten-salt corrosion experiments.

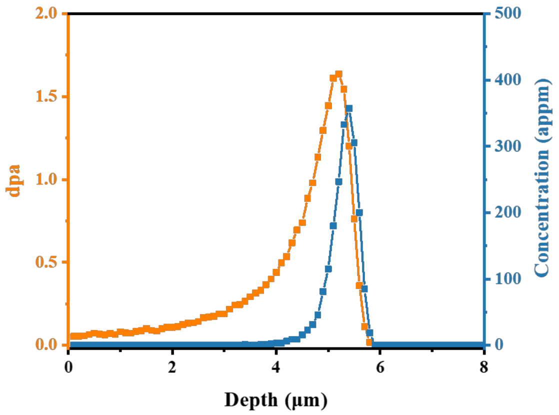

Figure. 2. SRIM-calculated dpa and Fe ion concentration profiles for the 1.06 MeV/u case

3. Conclusion

This work defined Fe ion irradiation conditions for MSR structural material Hastelloy N within the KAHIF operating conditions and used SRIM calculations to quantify and characterize the depth-dependent distributions of displacement damage and implanted Fe. Under RFQ-based conditions, the calculations indicate a subsurface maximum in the damage profile and a localized implantation region at slightly greater depths. Fluence scaling was used to construct a stepwise damage matrix while preserving the same depth distribution, enabling systematic comparison across damage levels. An additional higher-energy case based on IH acceleration shifts both the damage and implantation peaks to greater depths, extending the accessible damage-depth range. Overall, the calculated descriptors provide a consistent basis for specifying irradiation damage states and selecting analysis depth ranges for subsequent experimental studies.

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