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# Role of Heterogeneity in Manganese and Nickel Rich Precipitate Distribution on Hardening of Reactor Pressure Vessel Steels: Integrated Modeling and Experimental Characterization

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**ABSTRACT:**

Neutron irradiation induced embrittlement in reactor pressure vessel (RPV) steels is a critical issue for predicting and extending reactor lifetimes. RPV steel embrittlement is caused primarily by the irradiation assisted formation of stable matrix features, Cu rich precipitates (CRPs) and Mn-Ni rich precipitates (MNPs). CRPs form at low fluence in certain RPV steels, whereas MNPs nucleate and grow only at high fluence, likely due to their slow nucleation and growth kinetics. The role of MNPs is not included in most mechanistically based correlations (MBCs) for assessing RPV lifetimes and thus these models underestimate embrittlement at high neutron fluence. Experiments show that MNP distribution is heterogeneous near dislocation lines. Thus, the hypothesis of this work is that the different nucleation and coarsening kinetics of MNPs compared to CRPs, and the heterogeneous distribution of MNPs, both lead to unique hardening behavior at high neutron fluence. Ultimately, if the roles of MNP nucleation, growth and distribution on hardening and embrittlement are understood, including uncertainty, improved lifetime predictions for RPVs can be made.

The objective of this work is to understand hardening in RPV steels caused by MNPs via integrated multiscale modeling and experiments. Specifically, discrete dislocation dynamics (DDD) simulations will be performed to study mechanisms associated with dislocation interactions with MNPs and to extract yield stresses for a dislocation network with a heterogeneous distribution of MNPs. The focus of the DDD simulations will be on how MNP heterogeneity influences uncertainty in the yield stress shift. The distribution of MNPs at or near dislocation lines and prismatic dislocation loops in the DDD model will be guided by atomic kinetic Monte Carlo (AKMC) modeling, parameterized by Calphad models and density functional theory (DFT) calculations. This will provide volume fraction and the distribution of sizes of heterogeneously nucleated and coarsened MNPs. Experiments will be conducted on irradiated RPV steel samples and are designed to address a major challenge associated with the development of a high fluence embrittlement prediction model – lack of experimental data at extended life fluences. In addition, characterization and microscale mechanical testing will provide data necessary as input and validation of the computational models, specifically, information on the distribution of MNPs in samples irradiated to varying fluences at different temperatures, and the relationship between MNP density and mechanical properties of the RPV steels.

The deliverables of this work include: (i) quantification of MNP distribution during nucleation, growth and coarsening using AKMC simulations and both heterogeneity and distribution of MNPs in real neutron irradiated RPV samples via experiments; (ii) elucidation of the mechanisms behind MNP related hardening, including the change in yield stress and its uncertainty, using a combined DDD-experimental approach; and (iii) proposed advancement pathways for MBC models for hardening and embrittlement so that they account for heterogeneity in MNP distribution.