A Multiscale Approach to Understanding the Fundamental Mechanisms of Precipitation Strengthening in Steels

Thesis submitted to the

Indian Institute of Technology Kharagpur

for award of the degree

of

Doctor of Philosophy

by

Sankalp Biswal

(19MT91R20)

Under the guidance of

Prof. Debalay Chakrabarti and **Prof. Amlan Dutta**

Department of Metallurgical and Materials Engineering

Indian Institute of Technology Kharagpur

June 2026

Abstract

The present thesis adopts a multiscale approach to investigate the fundamental mechanisms governing precipitation strengthening, precipitate evolution, and their influence on the mechanical properties of advanced steels. Precipitation strengthening is one of the most sought-after mechanisms for improving the strength of materials and is primarily controlled by dislocation-precipitate interactions. Therefore, a detailed understanding of the precipitate evolution and dislocation-precipitate interaction mechanisms is essential for reliable prediction of strengthening behaior and rational alloy design. In this context, a combined atomistic modeling and experimental approach is employed. Atomistic and mesoscale simulation techniques such as molecular dynamics (MD), density functional theory (DFT), and discrete dislocation dynamics (DDD) are utilized to elucidate dislocation-precipitate interaction mechanisms, precipitate stability, and precipitation strengthening behavior. These simulations are complemented by experimental characterization techniques, which provide essential inputs parameters and enable validation of the computational predictions. The present work integrates multiscale simulations with experimental investigations to systematically study precipitation processes and associated strengthening mechanisms in three technologically important steel systems: Cu-added austenitic stainless steel forming Cu-rich precipitates during ageing, Fe-Ni-Ti ternary alloys containing η-Ni_3Ti precipitates in a BCC Fe matrix, and W-containing maraging steel, which shows a complex precipitation process. The three systems represent diverse combinations of matrix structure, precipitate chemistry and morphology, enabling systematic investigation of precipitation strengthening across different steels.

In the first alloy system, interactions of edge and screw dislocations with copper precipitate in an austenitic matrix were investigated. MD simulations revealed that for both edge and screw dislocations, the maximum value of strength was achieved when the dislocation exited the precipitate, indicating an attractive interaction between the dislocation and the precipitate. In the case of edge dislocation, the mechanism controlling the precipitation strengthening was found to be trailing partial detachment or leading partial detachment, depending on the precipitate size. On the other hand, for screw dislocations, numerous instances of dislocation recombination into constrictions were observed within the precipitate, whose probability increased with increasing precipitate size. Consequently, screw dislocation-precipitate interactions resulted in higher strengthening than edge dislocation interactions, primarily due to the repeated formation of constrictions. Besides, modulus strengthening was identified as

the primary strengthening contributor for the coherent Cu precipitate in the present alloy, which was subsequently aligned with the theoretical predictions by the existing Russell-Brown (R-B) model, adopting some modifications. The results were subsequently validated through DDD simulation and TEM analysis, providing a good corroboration with the experimental data. The present study provides valuable insights into the atomic-scale mechanism of precipitation strengthening in austenitic stainless steel.

In the second system, the dislocation-precipitate interactions and strengthening contributions of η-Ni_3Ti precipitates in BCC Fe was investigated using a coupled MD-DDD approach. MD simulations showed shearing of the precipitate by the edge dislocation, irrespective of the precipitate orientation. The mechanism of interaction, however, depended on the orientation of the precipitate basal planes relative to the slip plane of the matrix. In addition, the formation of stacking faults was also observed for certain precipitate variants. These results were complemented by transmission electron microscopy (TEM) observations in aged Fe-Ni-Ti alloys, demonstrating precipitate shearing and stacking fault formation within the precipitates. Further, DDD simulations, informed by inputs from MD simulations, were performed for different experimental precipitate distributions. These led to the development of suitable models that predicted the η-Ni_3Ti precipitation strengthening, consistent with the experimental results. In summary, this work, for the first time, investigated atomic-scale dislocation interactions with needle-shaped precipitates in maraging steels, supported by experimental evidence and extended to model strengthening due to random precipitate distributions.

All the Fe-Ni-Ti-based maraging steels typically contain significant amounts of other alloying elements (such as Co, Mo, W, Al, etc.). These elements partition either into the matrix or precipitate phases, affecting the precipitate stability as well as precipitation kinetics and mechanical properties. Subsequently, a commercial-grade W-containing maraging steel was systematically investigated to elucidate elemental partitioning behavior and precipitate evolution during ageing. TEM and APT analyses revealed the formation of fine η-Ni_3Ti precipitates containing significant amounts of Fe, Co, W, and Mo, along with W-Mo-rich clusters, indicating a complex precipitation process. DFT calculations revealed that W and Mo preferentially occupy Ti sites in η-Ni_3Ti, while Fe and Co favor Ni sites, explaining the experimentally observed partitioning. Ageing studies revealed a precipitation sequence involving initial Ni-Ti clustering, transient W-Mo incorporation into η-Ni_3Ti, and subsequent formation of a W-Mo-rich interfacial phase that evolves toward $(Fe,Ni)_2(W,Mo)$. DSC analysis

further revealed that W retards precipitation kinetics in maraging steels. The resulting microstructural evolution exhibited a strong correlation with mechanical behavior, leading to pronounced precipitation strengthening and a peak yield strength of approximately 2400 MPa. Overall, the present thesis establishes a unified multiscale framework that links atomic-scale mechanisms, experimentally determined precipitate sizes and distributions, precipitate chemistry, and microstructural evolution to macroscopic strengthening, providing a robust basis for the design and optimization of precipitation-hardened steels.

Keywords: Precipitation; Precipitation strengthening; Dislocations; Dislocation-precipitate interactions; Steel; Molecular dynamics simulations; Density functional theory; Discrete dislocation dynamics simulations