NEXT Competence Centre | Associated project Master thesis

Modeling TWIP and TRIP in Fe-Cr-Ni Alloys: A Crystal Plasticity (CP) Approach

Background

Austenitic Fe-Cr-Ni stainless steels exhibit exceptional mechanical properties through complex deformation mechanisms that depend critically on their metastable microstructural state. These alloys can undergo multiple competing plasticity mechanisms including dislocation slip, twinning-induced plasticity (TWIP), and transformation-induced plasticity (TRIP) involving strain-induced martensitic transformation from γ-austenite to α'-martensite. The activation of these mechanisms is governed by e.g. the stacking fault energy (SFE) and grain size, which control the thermodynamic and kinetic barriers for twin formation and phase transformation. At low SFE values (< 20 mJ/m^2), α'-martensite formation dominates, while intermediate SFE values (20-40 mJ/m^2) promote mechanical twinning, and high SFE (> 45 mJ/m^2) favors conventional dislocation glide. The competition between these mechanisms directly influences the strain hardening behavior and mechanical properties of the material.

Wong et al. (2016, Acta Mat.) developed a crystal plasticity (CP) model to predict ε-martensite and twin volume fractions based on SFE and grain size dependencies. Several studies (Jang et al. (1995, Mat. Char.), Tien et al. (2017a,b)) have demonstrated that ε-martensite serves as a precursor phase for α'-martensite formation through the sequential transformation pathway γ→ε→α', while mechanical twins provide nucleation sites for α'-martensite via shear band intersections. Recent studies by Galindo-Nava & Rivera-Diaz-del-Castillo (2017, Acta Mat.) and Benzing et al. (2019, Acta Mat.) established empirical relationships between ε-martensite nucleation rates and α'-martensite formation, while the Olson-Cohen model (1972, 1975) quantified α'-nucleation at twin boundary intersections. These relationships can be exploited to predict the effect of grain size and SFE on α'-martensite fractions based on the volume fraction of twins and ε-martensite.

Aims and objectives

This research aims to develop and validate an empirical postprocessing methodology for Fe-Cr-Ni alloys to predict α'-martensite evolution from twin and ε-martensite fractions using the TWIP/TRIP CP model developed by Wong et al. (2016, Acta Mat.). The specific objectives are: (1) determine the ε-martensite and twin volume fraction from CP simulations and apply empirical relations to predict α'-martensite fractions; (2) calibrate model parameters using experimental tensile testing data for four different grain size distributions through optimization approaches; (3) compare predictions of α'-martensite fraction evolution and lattice strain development against in-situ synchrotron HEXRD measurements; and (4) quantify the effects of grain size on critical stress thresholds for α'-martensite transformation initiation, providing empirical design guidelines for controlling deformation mechanisms in Fe-Cr-Ni alloys.

Activities and project timeline

Activity	2026				
	January	February	March	April	May
1. Literature review					
2. Model Calibration					
3. Empirical Postprocessing Methodology					
4. Crystal Plasticity Simulations					
5. Results Analysis					
6. Reporting					

Starting date: January 2026 or as agreed.

Duration: 5 months

Location: KTH

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