A multi-scale modelling of 3rd generation advanced high strength steels to account for anisotropic evolution of yield surface and plastic potential

Taejoon Park¹, Hyunki Kim¹, Ill Ryu², Farhang Pourboghrat¹, and Rasoul Esmaeilpour¹

¹ Department of Integrated Systems Engineering, The Ohio State University, 210 Baker Systems, 1971 Neil Avenue, Columbus, OH 43210, USA
² The Erik Jonsson School of Engineering & Computer Science, The University of Texas at Dallas, 800 West Campbell Rd., Richardson, TX 75080-3021, USA
E-mail: park.2417@osu.edu and pourboghrat.2@osu.edu (corresponding author)

Abstract. Multi-scale models were integrated to account for anisotropic mechanical behaviour of the 3rd generation advanced high strength steels (3GAHSS). The micromechanical response of individual phases of the 3GAHSS in non-proportional loading was characterized based on the atomistically informed dislocation dynamics (DD) simulations. The characterized mechanical properties were utilized for the development of the crystal plasticity model to properly account for the cross-loading effect on the interactions of the dislocations. To predict anisotropic evolution of yield surface and plastic potential in non-proportional loading of the 3GAHSS, 3D representative volume elements (3D RVEs) were developed based on the microstructural information from the EBSD data. As for the practical applications such as predictions of formability and spring-back, an advanced phenomenological model was also developed based on a combined type nonlinear isotropic-kinematic hardening law and two-yield surface plasticity.

1. Introduction
In the automotive industry, the demand for the advanced high strength steels (AHSS) is gradually increasing for better crashworthiness as well as the reduction in the vehicle weight. Recently, attentions have been focused on the development of 3rd generation advanced high strength steels (3GAHSS) due to their improved performance compared with the first generation of AHSS, and their economic advantages compared with the second generation of AHSS [1, 2]. In response to the introduction of the new 3GAHSS, advanced constitutive laws have been developed to improve the numerical prediction capability of finite element models for such parameters as formability and spring-back of stamped metal sheets.

In this study, multi-scale models were integrated to account for the mechanical behavior of the 3rd generation advanced high strength steels (3GAHSS). For the demonstration of the multi-scale modeling, an AHSS steel with 980 MPa grade tensile strength was considered, which was produced by the quenching and partitioning (Q&P) process; hereinafter the steel is referred to as Q&P980 steel.

2. Crystal plasticity model with dislocation density hardening based hardening law

2.1. Rate-independent crystal plasticity model
In order to account for the mechanical behavior of the 3GAHSS at microscale, the rate-independent crystal plasticity model, which was developed by Zamiri and Pourboghrat [3], was considered in this study. In the rate-independent crystal plasticity model, a yield surface is defined for a single crystal:

\[ f(\sigma) = \frac{1}{\rho} \ln \left( \sum_{\alpha=1}^{N} \exp \left( \frac{\rho}{m} \left( \frac{\sigma \cdot P^\alpha}{\tau^\alpha} - 1 \right) \right) \right) \]  

(1)

Here, \( \sigma \) is the Cauchy stress tensor, \( \tau^\alpha \) is the critical resolved shear stress (CRSS) on the slip system \( \alpha \), \( \rho \) and \( m \) are parameters for flexible control of the yield function shape, and \( P^\alpha \) is a symmetric matrix to define the slip system \( \alpha \):

\[ P^\alpha = \frac{1}{2} \left[ m^\alpha \otimes n^\alpha + (m^\alpha \otimes n^\alpha)^T \right] \]  

(2)

where \( n^\alpha \) is a unit normal direction vector to the slip plane, and \( m^\alpha \) is a unit slip direction vector.

2.2. Dislocation density based hardening evolution law

The critical resolved shear stress, \( \tau^\alpha \), can be assumed to be dependent on the density of dislocations \( f^\alpha \) [4]. By assuming that \( f^\alpha \) is mainly contributed by the forest dislocations, and \( f^\alpha_{\text{forest}} \) can be represented as the summation of the interactions:

\[ \tau^\alpha_{\text{forest}} = \mu b^\alpha \sqrt{\sum_{\beta=1}^{N} h^{\alpha\beta} f^\beta} \]  

(3)

where \( h^{\alpha\beta} \) is the matrix to generalize the forest dislocation interactions. The diagonal components of the matrix describe the interaction within the same slip systems, while the off-diagonal components represent the interactions between the different slip systems [5]. Lee et al. [6] proposed an interaction matrix based on the angle between the slip plane normal of the slip system \( \alpha \) (\( n^\alpha \)) and the line direction of the corresponding forest dislocation of the slip system \( \beta \) (\( \xi^\beta \)):

\[ h^{\alpha\beta} = n^\alpha \cdot \xi^\beta \]  

(4)

As for the evolution of the dislocation density \( f^\alpha \) of the slip system \( \alpha \), Kocks’ evolution law [7] was considered:

\[ df^\alpha = \frac{1}{b^\alpha} \left( \sqrt{\sum_{\beta=1}^{N} D^{\alpha\beta}} - k^\alpha \rho^\alpha \right) dy^\alpha \]  

(5)

Here, \( k^\alpha \) and \( k^\alpha \) are parameters to control the generation, evolution and annihilation of dislocation density.

3. Isotropic-kinematic hardening model based on two-yield surface plasticity

As for the phenomenological description of the mechanical behavior of the 3GAHSS at continuum scale, an isotropic-kinematic hardening model based on two-yield surface plasticity was considered. In the two-yield surface model, the conjugate stress, \( \Sigma \), and the back-stress, \( A \), define the (outer) bounding surface:

\[ f(\Sigma - A) - \Sigma_m^\alpha(\bar{\sigma}) = 0 \]  

(6)

The stress, \( \sigma \), on the (inner) yield surface and the corresponding stress, \( \Sigma \), on the (outer) bounding surface share the same direction so that,
where $\bar{\sigma}_{iso}$ and $\Sigma_{iso}$ are the effective sizes of the yield and bounding surfaces, respectively.

As for the back-stress evolution of the inner and outer surfaces,

$$dA = h_{z,\text{bound}} \left[ \rho_{z,\text{bound}} \left( \sigma - \sigma_{iso} \right) - A \right] d\varepsilon = h_{z,\text{bound}} \left[ \rho_{z,\text{bound}} \left( \Sigma - A \right) - A \right] d\varepsilon$$

and

$$da = h_{z,\text{inner}} \left[ \lambda \left( \sigma - \sigma_{iso} \right) - \alpha \right] d\varepsilon$$

respectively. The pseudo-equivalent quantity, $\bar{h}_{z,\text{bound}}$, and the non-equivalent quantities, $h_{z,\text{bound}}$ and $h_{z}$, are functions of the accumulative equivalent plastic strain, $\varepsilon$. For the constitutive modeling of the phase transformation from the retained austenite to martensite, the lattice deformation, the lattice-invariant shear deformation, and the orientation relationship between the parent austenite and transformed martensite were considered.

The relative motion of the yield surface with respect to the bounding surface is controlled by,

$$f(\Sigma - \sigma + \alpha - \bar{\Sigma}^m) = 0$$

4. Prediction of mechanical behaviour using a 3D representative volume element

A 3D representative volume element (3D RVE) for the Q&P980 steel was generated by using Dream3D software based on the raw EBSD data as shown in Figure 1. For the analysis of the distributions of grain size, grain shape, crystal orientation and misorientation from the EBSD data, MTEX Matlab toolbox software was utilized.

The generated 3D RVE was implemented into ABAQUS/Explicit FE solver by developing numerical scripts to assign the analysed microstructural information to individual elements. For verification, FE simulations for the uniaxial tension and uniaxial tension-compression tests were performed using the generated 3D RVE. As shown in Figure 2 (a), the stress-strain curve for the uniaxial tension was predicted closely by the CPFE simulation compared with the experimental result. Figure 3 (a) and (b) show the von Mises effective stress distributions of the deformed 3D RVE after elongation of 6.0%, followed by a compression of 12.0% during the uniaxial tension-compression test, respectively.
The CPFE simulation result for the uniaxial tension-compression test was utilized for the calibration of the two-yield surface model. Figure 2 (b) compares the CPFE simulation result in the uniaxial tension-compression test with the continuum scale FE simulation result based on the calibrated two-yield surface model.

![Figure 2](image)

**Figure 2.** Comparison of the stress-strain curves: (a) CPFE simulation and experimental results for the uniaxial tension test, and (b) CPFE simulation result in the uniaxial tension-compression test and calibration result for the two-yield surface model.

Based on the two-yield surface plasticity model, which was calibrated from the CPFE simulation result, the stress-strain curves in the uniaxial tension-compression-tension (T-C-T) test were predicted by performing the FE simulations at continuum scale. Figure 4 compares the stress-strain curves in the uniaxial T-C-T tests with various pre-strain histories. The uniaxial T-C-T tests were performed with an anti-buckling device, which was developed by Dr. Fadi Abu-Farha at Clemson University to prevent buckling of the specimen. Although the two-yield surface model was calibrated using only the CPFE simulation results excluding the experimental data, it can be confirmed that the FE simulation results are in good agreement with the experimental results in the uniaxial T-C-T test.

The asymmetry between tension and compression, which is also called strength differential (SD) effect [8], was observed in the Q&P980 steel. The SD effect was accounted for in the crystal plasticity model by adopting stress-state dependent martensitic phase evolution law [9]. As for the two-yield surface plasticity based phenomenological model, asymmetric yield function was adopted, and its evolution and kinematic translation were controlled to satisfy the consistency condition [10].
Figure 4. Comparison of the stress-strain curves in the uniaxial tension-compression-tension (T-C-T) test: FE simulation results based on the two-yield surface model and measured uniaxial T-C-T curves in the experiments.

5. Conclusions
Multi-scale models were integrated to account for the mechanical behavior of the 3rd generation advanced high strength steels (3GAHSS). A rate-independent crystal plasticity model with a dislocation density based hardening law was utilized to represent the mechanical behavior at the microscale, while a phenomenological model based on the two-yield surface plasticity was considered for the practical applications of the 3GAHSS steels at continuum scale. A 980 MPa grade Q&P steel was considered for the multi-scale modeling in this study. The hardening of the slip systems and the interactions between dislocations were calibrated based on in-situ X-ray diffraction (HEXRD) tensile test data and atomistically informed dislocation dynamics (DD) simulation results, respectively. A 3D RVE was generated for the Q&P980 steel by using Dream3D and MTEX Matlab toolbox software based on the EBSD data. Although the phenomenological two-yield surface model was calibrated using only the CPFE simulation results excluding the experimental data, the stress-strain curves in the uniaxial tension-compression-tension (T-C-T) test were predicted very closely by the FE simulations with the two-yield surface model compared with the experimental results.

Acknowledgments
This material is based upon work supported by the Department of Energy under Cooperative Agreement Number DOE DE-EE000597, with United States Automotive Materials Partnership LLC (USAMP).

References
[1] Matlock D K and Speer J G 2009 Microstructure and Texture in Steels: and Other Materials, ed A Haldar, et al. (London: Springer London) pp 185-205
[2] De Moor E, Gibbs P, Speer J, Matlock D and Schrot J 2010 Iron & steel technology 7 132
[3] Zamiri A R and Pourboghrat F 2010 Int J Plasticity 26 731-46
[4] Ardelen M, Beyerlein I J and Knezevic M 2014 J Mech Phys Solids 66 16-31
[5] Beyerlein I J and Tomé C N 2008 Int J Plasticity 24 867-95
[6] Lee M G, Lim H, Adams B L, Hirth J P and Wagoner R H 2010 Int J Plasticity 26 925-38
[7] Kocks U F 1976 J Eng Mater Tech 98 76-85
[8] Maeda T, Noma N, Kuwabara T, Barlat F and Korkolis Y P 2018 J Mater Process Tech 256 247-53
[9] Beese A M and Mohr D 2011 Acta Materialia 59 2589-600
[10] Chung K and Park T 2013 Int J Plasticity 45 61-84