An integrated computational materials engineering approach for constitutive modelling of 3rd generation advanced high strength steels

Farhang Pourboghrat¹, Taejoon Park¹, Hyunki Kim¹, Bassam Mohammed¹, Rasoul Esmaeilpour¹ and Louis G. Hector, Jr.²

¹ Department of Integrated Systems Engineering, The Ohio State University, 210 Baker Systems, 1971 Neil Avenue, Columbus, OH 43210, USA
² GM R&D Center, General Motors Corporation, Warren, MI 40890, USA
E-mail: pourboghrat.2@osu.edu, park.2417@osu.edu, and louis.hector@gm.com

Abstract. Constitutive models for the 3rd generation advanced high strength steels (3GAHSS) were developed based on integrated computational materials engineering (ICME) approach. Multiple scale models from the atomic level to the continuum level were integrated to generate material models that can be used to accurately model the material response of the 3GAHSS depending on their microstructures. In addition to the shear deformation in the slip systems, martensitic phase transformation induced by the plastic deformation of the retained austenite was accounted for in the crystal plasticity model. Atomistic simulation results based on the density functional theory (DFT) calculations were utilized to obtain the lattice parameters and elastic coefficients, while micropillar compression data and in-situ HEXRD test data were utilized for the characterization of the developed crystal plasticity model. 3D representative volume elements (RVE) were generated to represent the mechanical behaviour of the 3GAHSS by considering the distributions of grain size, grain shape, and grain orientation measured from the EBSD data. To predict macroscopic mechanical behaviour of 3GAHSS in complex deformations, finite element simulations were performed based on the developed crystal plasticity model and generated 3D RVEs. The CPFE simulation results were implemented in the advanced phenomenological models and utilized to accurately predict the formability and spring-back of 3GAHSS.

1. Introduction
The 3rd generation advanced high strength steel (3GAHSS) is a composite material designed to have complex microstructures comprised of phases with high strength and ductility. The improved strength is achieved with fine-grained ferrite, martensite, or bainite, while the retained austenite enhances ductility by introducing martensitic phase transformation. Therefore, it is crucial to understand the microstructure-induced mechanical behavior of the material to optimize the material performance of 3GAHSS.

A 3GAHSS steel (Fe-0.3C-3.0Mn-1.6Si, wt.%) with a 1500 MPa grade tensile strength, which was developed by AK Steel Corporation and CANMET Materials (CMAT), was considered in this work. The steel was produced by the quenching and partitioning (Q&P) process; hereinafter the steel is referred to as Q&P1500 steel. The Q&P1500 steel contains 17.5 % volume fraction of retained austenite and balanced martensite (57.5 vol.% for the tempered martensite and 25.0 vol.% for the untempered martensite). In the uniaxial tensile test, the engineering uniform elongation limit, the 0.2% offset initial
yield, and the ultimate tensile engineering strength of the Q&P 1500 steel were found to be 12%, 1270 MPa, and 1500 MPa, respectively.

2. Rate-independent crystal plasticity model
A combined yield function is defined for a single crystal in the rate-independent crystal plasticity model developed by Zamiri and Pourboghrat [1]:

\[ f(\sigma) = \frac{1}{\rho} \ln \left( \sum_{\alpha=1}^{\infty} \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\alpha}{\tau_y^\alpha} - 1 \right) \right] \right) \]  

(1)

Here, \( \sigma \) is the Cauchy stress tensor, \( \rho \) and \( m \) are parameters for flexible control of the yield function shape, \( \tau_y^\alpha \) is the critical resolved shear stress (CRSS) on the slip system \( \alpha \), 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 to the slip plane, and \( m^\alpha \) is a unit slip direction.

The rate of plastic deformation tensor is derived from equation (1) based on the normality rule:

\[ D^p = \lambda \frac{\partial f(\sigma)}{\partial \sigma} = \lambda \frac{\sum_{\alpha=1}^{\infty} \text{sign}(\sigma : P^\alpha) \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\alpha}{\tau_y^\alpha} - 1 \right) \right] P^\alpha}{m \sum_{\beta=1}^{\infty} \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\beta}{\tau_y^\beta} - 1 \right) \right]} \]  

(3)

where \( \lambda \) is Lagrange multiplier. Since the plastic deformation is defined as,

\[ D^p = \sum_{\alpha=1}^{\infty} \dot{\gamma}^\alpha P^\alpha \]  

(4)

The shear strain rate \( \dot{\gamma}^\alpha \) is derived from equation (3):

\[ \dot{\gamma}^\alpha = \lambda \frac{\sum_{\alpha=1}^{\infty} \text{sign}(\sigma : P^\alpha) \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\alpha}{\tau_y^\alpha} - 1 \right) \right] P^\alpha}{m \sum_{\beta=1}^{\infty} \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\beta}{\tau_y^\beta} - 1 \right) \right]} \]  

(5)

The spin tensor is defined as,

\[ \Omega^p = \sum_{\alpha=1}^{\infty} \dot{\gamma}^\alpha w^\alpha \]  

(6)

By substituting the shear strain rate in equation (5),

\[ \Omega^p = \lambda \frac{\sum_{\alpha=1}^{\infty} \text{sign}(\sigma : P^\alpha) \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\alpha}{\tau_y^\alpha} - 1 \right) \right] w^\alpha}{m \sum_{\beta=1}^{\infty} \exp \left[ \frac{\rho}{m} \left( \frac{\sigma : P^\beta}{\tau_y^\beta} - 1 \right) \right]} \]  

(7)

Here, \( w^\alpha \) is a skew-symmetric matrix conjugate to the symmetric matrix \( P^\alpha \).
3. Martensitic phase transformation model

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.

3.1. Phenomenological description

The lattice deformation of the retained austenite is called Bain deformation as schematically shown in Figure 1 and its deformation gradient matrix, $B$, has the following form in the coordinate system for the FCC lattice,

$$
(B)_{ij} = \begin{pmatrix}
\eta_1 & 0 & 0 \\
0 & \eta_2 & 0 \\
0 & 0 & \eta_3
\end{pmatrix}
$$

(8)

where $\eta_1$, $\eta_2$, and $\eta_3$ are the expansion ratio from the FCC lattice to BCT lattice.

In order to accommodate the orientation relationship between the parent austenite and product martensite, the rigid body rotation, $R$, is additionally needed to have at least one invariant-line. Also, the habit plane (interface between the parent austenite and product martensite) should be an undistorted and unrotated plane for the cooperative atomic movement during the martensitic transformation. Therefore, the complementary lattice-invariant shear deformation is additionally considered for the phenomenological description of the martensitic phase transformation [2]. The macroscopic deformation gradient tensor, $P_1$, is obtained by the rigid body rotation, Bain distortion, and complementary invariant shear deformation, $P_2$ [3, 4]:

$$
P_1 = RBP_2^{-1}
$$

(9)

3.2. Phase volume fraction evolution

The following empirical evolution law, which was developed by Beese and Mohr [5], was adopted for the Q&P1500 steel:

$$
\dot{f}_m = (f_m^{\text{max}} - f_m) n D \bar{\varepsilon}^{n-1}
$$

(10)

Here, $\bar{\varepsilon}$ is the equivalent plastic strain, $f_m$ is the volume fraction of the transformed martensite, $f_m^{\text{max}}$ is the maximum volume fraction, $n$ and $D$ are the material parameters to control the rate of the transformation.

4. Material characterization

The lattice parameters and elastic coefficients for each phase in the Q&P1500 steel were calculated based on the solute and temperature dependent mesoscale models developed by Fellinger et al. [6].

The evolution of the retained austenite volume fraction in the Q&P 1500 steel was measured by in-situ synchrotron based high-energy X-ray diffraction (HEXRD) tensile test. The diffraction of the high-energy synchrotron X-ray beamline was measured at 11 I-D-C, at the Advanced Photon Source (APS), Argonne National Laboratory (ANL). The tensile specimens with the gauge length of 10 mm were prepared along the rolling direction (RD). The tensile tests were carried out at a constant grip speed of 30 µm/s at room temperature. From the generated Debye rings during the in-situ tensile test, lattice strain
for each phase of the Q&P 1500 steel were measured and provided by Pacific Northwestern National Laboratory (PNNL) [7].

An empirical model was developed to calculate the phase stress from the lattice strain histories by considering iso-stress (lower bound) and (semi) iso-strain (upper bound) conditions. The calibrated phase stress histories with respect to the macroscopic strain are compared to the CPFEM simulation results in Figure 3.

![Figure 2](image1.png)

**Figure 2.** Measured volume fraction evolution of the retained austenite during the in-situ uniaxial tensile test.

![Figure 3](image2.png)

**Figure 3.** Comparison of the calibrated and simulated macroscopic stress strain curves during the in-situ uniaxial tensile test.

5. **Finite element simulations with a 3D representative volume element**

From the measured EBSD data, microstructural information of the Q&P1500 steel such as distributions of grain size, grain shape, orientation and misorientation was analysed using MTEX Matlab toolbox software. Then, a 3D representative volume element (RVE) was generated by utilizing Dream3D software based on the calibrated microstructural information as shown in Figure 4.

![Figure 4](image3.png)

**Figure 4.** Generated 3D RVE for the Q&P1500 steel: (a) Phase distribution and (b) Crystal orientation distribution.

A finite element simulation for the uniaxial tensile test was performed using the developed constitutive law and the generated 3D RVE for the Q&P1500 steel. Figure 5 shows the deformed 3D RVE with the von Mises effective stress distribution and maximum principal strain distribution after performing the uniaxial tension simulation up to 12.5% engineering strain, and Figure 6 compares the simulated and
experimentally measured engineering stress-strain curves. The initial yield stress, uniform elongation limit, and the overall stress-strain curve shape were predicted to be very similar to the experimental results.

Figure 5. Deformed 3D RVE after performing the uniaxial tension simulation: (a) von Mises effective stress distribution and (b) maximum principal strain distribution.

Figure 6. Comparison of the measured and simulated stress-strain curves for the Q&P1500 steel in the uniaxial tension test.

6. Conclusions
A constitutive law was developed for the mechanical behaviour of 3G AHSS based on an integrated computational materials engineering (ICME) approach. A strain-induced martensitic phase transformation model was developed based on the rate-independent crystal plasticity. A 1500 MPa grade Q&P steel was considered in this study and the mechanical properties of the retained austenite, pre-existing martensite, and newly formed martensite were calibrated by iteratively performing CPFE simulations based on the in-situ high energy X-ray diffraction (HEXRD) tensile test data. A 3D RVE was generated using Dream3D and MTEX Matlab toolbox software based on the microstructural information from the EBSD data such as the distributions of grain size, grain shape, and crystal orientation. For verification, CPFE simulations were performed for the uniaxial tensile test based on the developed material model and the generated 3D RVE. The prediction of initial yield stress, uniform elongation limit, and ultimate tensile strength are in good agreement with experiments.

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] Zamiri A R and Pourboghrat F 2010 International Journal of Plasticity 26 731-46
[2] Nishiyama Z, Fine M E and Wayman C M 1978 Martensitic transformation: Academic Press
[3] Mackenzie J K and Bowles J S 1954 Acta Metallurgica 2 138-47
[4] Wechsler M S, Lieberman D S and Read T A 1953 Trans. AIME 197 1503
[5] Beese A M and Mohr D 2011 Acta Materialia 59 2589-600
[6] Fellinger M R, Hector Jr L G and Trinkle D R 2017 Computational Materials Science 126 503-13
[7] Hu X, Choi K S, Sun X, Ren Y and Wang Y 2016 Metallurgical and Materials Transactions A 47 5733-49