**3.1 Rate dependent material models for ferrite, martensite and retained austenite in Q&P980 steel**

Q&P980 steel contains three phases: ferrite, martensite, and retained austenite. Crystal plasticity models for each phase were developed and calibrated using micro-pillar indentation data in ref. [2]. The crystal plasticity models cannot be used directly to model fracture, because they do not account for failure. Instead, fracture simulations use isotropic hardening models for each phase, whose properties are computed by simulating the behavior of ‘virtual’ polycrystals.

The elastic behavior of all three phases were assumed to be identical, with Young’s modulus:  MPa; Poisson’s ratio: .

*Ferrite and Martensite Phases*

The Ferrite and Martensite phases are modeled using an isotropic rate-dependent plasticity model. Following the standard procedure, the strain rate (strictly, the symmetric part of the velocity gradient) is divided into elastic and plastic parts as



The elastic strain rate is related to stress rate by the usual isotropic elastic stress-strain law. The plastic strain rate is related to stress by



Here,  is the Cauchy (true) stress. The von-Mises effective uniaxial plastic strain rate  is related to Von-Mises stress by



Here, are two new material parameters, which describe the strain rate sensitivity of the material. This (and the equivalent extension for our model of retained Austenite described below) is the main new feature of the model that was implemented during the past quarter. The flow stress is related to accumulated von-Mises effective strain by:



where  is the initial flow stress; while *Q,b,H,n* are parameters that model strain hardening. Note the addition of a strain hardening exponent *n* in eq. which was not present in the model described last quarter. These parameters were calculated by first creating representative volume elements of polycrystalline ferrite and martensite, and calculating the uniaxial stress-strain curves for these ‘virtual’ materials. The predictions of equation were then fit to these predictions. The procedure is described in more detail (for DP steels) in the report for the previous quarter. The final set of material parameters is reported in Table 1: these data should be contrasted with corresponding results in Table 1 of the report for the prior quarter.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Phase** | (MPa) | (MPa) | (MPa) |  | *n* |  | *m* |
| Martensite | 780 | 350 | 525 | 370 | 1.0 | 0.21 | 0.01 |
| Ferrite | 540 | 1500 | 175 | 330 | 1.0 | 0.21 | 0.01 |

Table 1: Yield strength and hardening parameters of martensite and ferrite phases in Q&P980 steel.

The predicted nominal uniaxial stress-strain curve is compared with the simulated behavior of polycrystals of ferrite and martensite in Q&P980 in Fig. 1. We do not observe a significant difference between these results and the corresponding Fig 3. in the report for the previous quarter.

**Ferrite**

**Martensite**

**Isotropic RVE**

**CP RVE**

**Isotropic RVE**

**CP RVE**

**(a)**

**(b)**



1. (b)

Figure. 1: Comparison of the nominal stress versus strain curves predicted by crystal plasticity and isotropic RVEs for (a) ferrite and (b) martensite phases (CP – crystal plasticity).

*Retained Austenite Phase*.

Following a similar approach, we have also implemented a rate dependent model for the retained austenite in Q&P980 steel.

The total strain rate (the symmetric part of the velocity gradient) is decomposed into three contributions



Here,  is the elastic strain rate, which is related to stress rate by the usual linear elastic constitutive equations,  is the strain rate resulting from plastic deformation (slip) in the untransformed austenite and martensite (note that these are combined into a single term in this model, while the crystal plasticity model of RA transformation contains separate terms that describe plasticity from untransformed austenite and martensite), and  is the strain resulting from the change in lattice structure associated with the austenite to martensite transformation.

The plastic strain rate is related to the stress through eq. and , and we also use eq to describe strain hardening of the retained austenite, but instead of using constants, we take  to be material state variables, which evolve with the volume fraction of transformed austenite *z* as follows



where  represent flow stress and hardening parameters (constants) for single phase (untransformed) austenite, and  are the corresponding properties for single phase transformed martensite.

The martensite volume fraction is assumed to evolve with accumulated plastic strain and stress according to



Where the functions *A* and *B* are given by



where { } are material properties.

Finally, the transformation strain rate is taken to be



The constants  are material properties.

The material properties in this model are determined by computing the uniaxial stress-strain response of a ‘virtual’ polycrystal of retained austenite, which is modeled using the crystal plasticity formulation described and calibrated in ref. [2]. The material properties in the isotropic model are chosen to fit the predicted stress-strain curve and the evolution of the volume fraction of transformed austenite with strain. The relevant material parameters are listed in Table 2.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| (MPa) | (MPa) | (MPa) | (MPa) | (MPa) |  | *n* |  | *m* |
|  |  |  |  |  |  | 1.05 | 0.21 | 0.01 |

Table 2a: Hardening parameters of isotropic model of retained austenite

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| (1/MPa) | (1/MPa2) |  |  | (MPa) |
|  |  |  |  |  |

**Table 2b**: Transformation parameters of isotropic model of retained austenite

The predictions of the isotropic RA model are compared to the crystal-plasticity computations in Fig 2. The rate dependent model predicts behavior that is very similar to the rate independent formulation reported in the preceding quarter.

**Isotropic RVE**

**CP RVE**

**(a)**

**(b)**

**Isotropic RVE**

**CP RVE**



Figure 2: (a) comparison of the nominal stress versus strain curves predicted by crystal plasticity and isotropic RVEs for retained austenite and (b) evolution of martensite volume fraction during the deformation process.

*Flow behavior of 3D representative volume elements of Q&P980 steel*

As a further test of the isotropic model, a 3D representative volume element of Q&P980 microstructure was created following the procedure described in ref [2]. The phases were idealized using the approximate isotropic constitutive equations described in this section, and the nominal stress-strain response of the microstructure was computed. The predicted behavior is compared with experimental measurements in Fig 5. The isotropic model over-estimates the flow stress for strains below 5%, but thereafter matches experiments well. The rate-dependent constitutive equations give a much better match to the full crystal plasticity simulations than the rate independent formulation reported in the preceding quarter. In particular, note that the martensite volume fraction in Fig 3 (b) now gives excellent agreement with the full crystal plasticity model.



**Isotropic RVE**

**Experiment**



**CP RVE**

**Isotropic RVE**

**(a)**

**(b)**

Figure 3: (a) comparison of experimental nominal stress-strain predicted by calibrated isotropic RVE (Fe-50%; Ma-42%; RA-8%) with experimental stress-strain curve; (b) Variation of martensite volume fraction predicted by the isotropic and crystal plasticity models.