A new crystal plasticity modeling of uniaxial ratcheting behavior for face-centered cubic 6061 aluminum alloy

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Abstract
The uniaxial ratcheting behavior of face-centered cubic 6061 aluminum alloy is investigated theoretically based on the crystal plasticity theory. In this model, a simplified flow rule is adopted for convenient engineering application, and the classical Kocks-Mecking-Estrin isotropic hardening rule related to dislocation density is adopted to describe the cyclic hardening characteristic of the material. The classical Armstrong-Frederic kinematic hardening rule is modified associated with cumulative slip to predict the ratcheting behavior more accurately. The single crystal version of this model is expanded to metal polycrystalline using a simplified explicit scale transition rule. The capability of the proposed model to capture the uniaxial ratcheting response of metal polycrystalline is verified by comparing the predictions with the corresponding experimental results of 6061 aluminum alloy. The evolution of uniaxial ratcheting of 6061 aluminum alloy can be reasonably predicted by the proposed model, and the capability to simulate uniaxial ratcheting behavior in inter-granular scale is qualitatively discussed as well.

1. Introduction
The cyclic accumulation of plastic deformation, that is to say, ratcheting effect, often produces in engineering structure when it subject to asymmetrical stress cycling. The occurrence of ratcheting strain will lead to the deformation beyond the limit or fatigue life reduction. In the past four decades, many researchers have conducted a large number of experimental and corresponding cyclic constitutive model studies on the ratcheting behavior of various pure metal and alloy materials, as reviewed by Kang [1], Chaboche [2] and Sai [3]. The dependence of ratcheting behavior on mean stress, stress amplitude, stress ratio, ambient temperature and loading history have been extensively researched based on the systematic macroscopic experimental researches. Due to lack of experimental researches on microscopic mechanism of ratcheting, nearly all of theoretical researches were constructed directly by fitting the macroscopic experimental data [4]. The physical mechanism of ratcheting were not involved in these models, which results in an inaccurate prediction of the ratcheting deformation. As everyone knows, dislocation slip is the dominant deformation mechanism of plastic deformation of polycrystalline metals. Concerning the microscopic mechanism of ratcheting deformation, some pioneering investigations [5–7] for 316L stainless steel paid more attention to the final dislocation substructures formed at the end of the uniaxial/multiaxial ratcheting deformation, rather than the evolution of microscopic substructures in the ratcheting process. Recently, the microscopic substructure evolution during uniaxial/multiaxial ratcheting of face-centered cubic (FCC) 316L stainless steel [8, 9], body-centered cubic ordinary carbon steel [10, 11] and close-packed hexagonal Ti-6Al-4V [12] were observed systematically by the author and his co-workers. The physical mechanism of ratcheting deformation was qualitatively explained by the microscopic observations, and the heterogeneous dislocation patterns were the main mechanism of ratcheting. These works are very helpful to construct the cyclic constitutive model based on the physical mechanism.
Recently, some innovative researches were carried out to implant the physical mechanism of ratcheting into the theoretical models based on the multi-mechanism theory. Firstly presented by Cailletaud et al [13], the multi-mechanism model include some physical information, and can supply preferable predictions of ratcheting, as reviewed by Sai [3]. Nevertheless, the physical mechanism were not explicitly involved in the multi-mechanism models. As discussed by Kang and his co-workers [14, 15], crystal plasticity is a reasonable choice to implant the physical mechanism into the cyclic constitutive models. By introducing the modified Armstrong-Frederic kinematic hardening rule, the uniaxial/multiaxial ratcheting can be reasonably predicted for many kinds of engineering structural material [16–26]. However, for the sake of reflecting the physical mechanism of ratcheting deformation, plenty of internal variables and material parameters were involved in these models. Excessive material parameters limit the practical application of these models, and the cyclic ratcheting constitutive models suitable for engineering application are still need to develop.

As a result, take into consideration of the long-range interaction of dislocation in intra-granular scale, a revised Armstrong-Frederic kinematic hardening rule associated with cumulative slipping is employed to predict ratcheting more precisely. The cyclic hardening characteristic is described by a classical Kocks-Mecking-Estrin isotropic hardening rule related to dislocation density. Using a simplified explicit transition approach, the single crystal constitutive model is expanded to metal polycrystalline. Finally, the proposed model is verified by comparing the predict results with experimental ones of 6061 aluminum alloy. Simultaneously, the uniaxial ratcheting behavior of 6061 aluminum alloy single crystal is also qualitatively discussed here.

2. Constitutive model framework

2.1. Main equation in intra-granular scale

With small deformation hypothesis, the total strain tensor \( \varepsilon \) is directly decomposed into the elastic strain tensor \( \varepsilon^e \) and the viscoplastic strain tensor \( \varepsilon^p \) in the framework of crystal plasticity:

\[
\varepsilon = \varepsilon^e + \varepsilon^p
\]

(1)

Assuming a uniform stress-strain field in a single grain for briefness, we can assumed that dislocation slip do not affect the elastic properties. Therefore, the elastic strain tensor \( \varepsilon^e \) caused by the lattice distortion can be obtained by the fourth order elasticity tensor \( C \) and stress tensor \( \sigma \):

\[
\varepsilon^e = C : \sigma
\]

(2)

As everyone knows, the main inelastic deformation mechanism of FCC metals is dislocation slip, and the viscoplastic strain rate \( \dot{\varepsilon}^p \) can be represent as:

\[
\dot{\varepsilon}^p = \sum_{\alpha=1}^{n_{slip}} P^\alpha \dot{\gamma}^\alpha
\]

(3)

\[
P^\alpha = \frac{1}{2} (s^\alpha \otimes m^\alpha + m^\alpha \otimes s^\alpha)
\]

(4)

where \( P^\alpha \) and \( \dot{\gamma}^\alpha \) are the orientation tensor and slipping rate, respectively. The orientation tensor \( P^\alpha \) can be acquired by the slip direction vector \( s^\alpha \) and slip plane normal vector \( m^\alpha \) making use of equation (4). The slip system in FCC metals is \{111\} ⟨110⟩, and \( n_{slip} \) is the total number of active slip systems.

Considering a representative volume element within a single crystal, the Helmholtz free energy can be divided into elastic strain energy \( \psi^e \) and plastic hardening energy \( \psi^p \):

\[
\psi = \psi^e + \psi^p
\]

(5)

The elastic strain energy is denoted as the quadratic form of the elastic strain tensor as:

\[
\psi^e = \frac{1}{2} \varepsilon^e : C : \varepsilon^e
\]

(6)

while, the plastic hardening energy includes two parts, i.e., \( \psi^p_{iso} \) caused by isotropic hardening and \( \psi^p_{kin} \) caused by kinematic hardening. The rate forms of these two items can be express as equation (7) and equation (8):

\[
\psi^p_{iso} = \sum_{\alpha=1}^{n_{slip}} x^\alpha \tau^\alpha
\]

(7)

\[
\psi^p_{kin} = \sum_{\alpha=1}^{n_{slip}} \tau^\alpha \dot{\gamma}^\alpha
\]

(8)

where, \( x^\alpha \) and \( \tau^\alpha \) are the back stress and critical shear stress of slip system \( \alpha \), respectively. The second law of thermodynamics for isothermal process in per unit volume is:
\[ \sigma: \dot{\varepsilon} - \dot{\psi} \geq 0 \]  

Namely, the stress power of the representative volume unit is not less than the energy storage rate, and the dissipation per unit volume is non-negative. Substituting equations (1), (3) and (6) to (8) into equation (9) will lead to:

\[ \sigma: (\varepsilon^e + \varepsilon^p) - \frac{\partial \psi^e}{\partial \varepsilon^e} - \sum_{\alpha=1}^{nslip} \left( x^\alpha \gamma^\alpha - \tau^\alpha_i |\dot{\gamma}^\alpha| \right) \geq 0 \]  

The elastic stress-strain relationship can be derived from the thermodynamic equation of state:

\[ \sigma = \frac{\partial \psi^e}{\partial \varepsilon^e} = C: \varepsilon^e \]  

Substituting equation (11) into equation (10) can further get:

\[ \sigma: \sum_{\alpha=1}^{nslip} \dot{\gamma}^\alpha \mathbf{P}^\alpha - \sum_{\alpha=1}^{nslip} x^\alpha \dot{\gamma}^\alpha + \tau^\alpha_i |\dot{\gamma}^\alpha| \geq 0 \]  

Equation (12) requires that every slip system in a single crystal needs to satisfy the dissipation inequality of Clausius-Duhem form:

\[ \Gamma^\alpha = (\sigma: \mathbf{P}^\alpha - x^\alpha) \dot{\gamma}^\alpha - \tau^\alpha_i |\dot{\gamma}^\alpha| \geq 0 \quad (\alpha = 1, 2, \ldots, nslip) \]  

The first term of equation (13) must be non-negative if dissipation is non-negative, and it must satisfied:

\[ \text{sign}(\dot{\gamma}^\alpha) = \text{sign}(\sigma: \mathbf{P}^\alpha - x^\alpha) \]  

Making use of equation (14), the Clausius-Duhem dissipation inequality can be rewritten as:

\[ \Gamma^\alpha = |\sigma: \mathbf{P}^\alpha - x^\alpha| - \tau^\alpha_i \geq 0 \quad (\alpha = 1, 2, \ldots, nslip) \]  

Therefore, the thermodynamic driving force \( \pi^\alpha \) of conjugated with |\dot{\gamma}^\alpha| can be defined as:

\[ \pi^\alpha = |\sigma: \mathbf{P}^\alpha - x^\alpha| - \tau^\alpha_i \]  

Aim to reduce the material parameters to some extent, a simplified rate-dependent flow rule [27, 28] is adopted in this work:

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{|\tau^\alpha - x^\alpha|}{\tau^\alpha_i} \right)^m \]  

Where \( \dot{\gamma}_0 \) is the reference slipping rate in slip system \( \alpha \); \( m \) is the viscosity coefficient of the material.

### 2.2. Revised kinematic hardening rule

To better prediction of ratcheting response, a revised Armstrong-Frederick kinematic hardedning rule is proposed in this work. The rate form of back stress \( x^\alpha \) is outlined as:

\[ x^\alpha = g \dot{\gamma}^\alpha - h \alpha \dot{\gamma}^\alpha |\dot{\gamma}^\alpha| \]  

The first term in the kinematic hardening rule is a linear strengthening term related to dislocation proliferation and interaction, and \( g \) is the coefficient of the linear strengthening item. The second term is a dynamic recovery term associated with dislocation annihilation with a coefficient \( h \). As everyone knows, the classical Armstrong-Frederick hardening rule usually overestimate the ratcheting strain because of the excessive dynamic recovery effect [14]. Therefore, the coefficient of the dynamics recovery item \( b \) can be revised as:

\[ h = h_0 + (h_{sat} - h_0) \left( 1 - \exp \left( \frac{\gamma}{\gamma_0} \right) \right) \]  

where \( h_0 \) and \( h_{sat} \) are the original value and saturation value of \( h \); \( \gamma_0 \) and \( \gamma \) are the eference values of cumulative slip and cumulative slip in a single crystal, respectively. The cumulative slip \( \gamma \) can be obtained by integrating all active slip systems in a single crystal:

\[ \gamma = \sum_{\alpha=1}^{nslip} \int_0^t |\dot{\gamma}^\alpha| \, dt \]  

### 2.3. Dislocation density based isotropic hardening rule

The isotropic hardening related to the short-range interaction of dislocations can be described by the slip resistance of the slip system, using the following classical Kocks-Mecking-Estrin formula [29]:
\[ \tau_c^\alpha = \left[ \tau_c^{\alpha_0} + M \Omega_1 \mu b \sqrt{\rho^\alpha} \right] \left( \frac{\rho^\alpha}{\rho_0} \right) \]

where \( \tau_c^{\alpha_0}, M, b, \) and \( \mu \) are respectively the initial critical shear stress, Taylor factor, magnitude of the Burgers vector and shear modulus; \( \rho^\alpha \) is the dislocation density of slip system \( \alpha \).

According to the discussion by Estrin and Mecking [29], the dislocation density law is governed by:

\[ \dot{\rho}^\alpha = \left( \frac{1}{bL} - K_2 \rho^\alpha \right) M^{-1/2} \]

where, the free mean path of dislocation \( L \) decreases as the incrementally of dislocation interaction; \( K_2 \) is a material parameter related to dislocation annihilation. As discussed by Krishnaswamy and Barlat [30], the material parameter \( K_2 \) is governed by the following empirical equation accompanied by a proportional relationship between \( L \) and \( 1/\sqrt{\rho} \):

\[ K_2 = K_{2,0} \left( \frac{\rho}{\rho_0} \right)^{1/2} \]

in which \( n \) and \( K_{2,0} \) are material parameters related to the dislocation annihilation.

2.4. Explicit scale transition criterion

The above constitutive model is limited to intra-granular scale. To predict the ratcheting of polycrystalline metals in which intra-granular scale constitutive model is inapplicable, we need to introduce an efficient scale transition criterion. The self-consistent model proposed by Hill [31] is an excellent approach to acquire the polycrystalline aggregate response from single crystal. Nevertheless, the implicit algorithm is very complex and time-consuming. Therefore, in this work, a succinct explicit scale transition rule named \( \beta \)-rule [32] is accepted in this work. Based on the hypothesis of uniform elasticity of polycrystalline aggregate, the local stress tensor \( \sigma^\varepsilon \) is directly acquired from the macroscopic stress tensor \( \Sigma \) by:

\[ \sigma^\varepsilon = \Sigma + C (\beta - \beta^\varepsilon) \]

\[ \dot{\beta}^\varepsilon = \dot{\varepsilon}^p - D (\beta^\varepsilon - \varepsilon^p) \]

where, \( \beta = [\beta^\varepsilon] \) and the symbol \([ \cdot ]\) denotes the volume average over all the grains of the polycrystalline aggregations. \( C \) and \( D \) are material parameters. The proposed cyclic viscoplastic constitutive model compose of equations (1)–(25) is verified in the next section taking advantage of the experimental results of 6061 aluminum alloy.

3. Experimental results and model verification

3.1. Experimental materials and methods

In this work, FCC 6061 aluminum alloy is employed to verify the capability of the proposed model to predict the cyclic deformation responses. The chemical component of 6061 aluminum alloy is shown in table 1. After T6 heat treatment (Solution treatment and artificial aging), dumbbell-shaped specimens (gage length of 18 mm and diameter of 6 mm) was machined from solid bars, and a MTS809-250KN material testing machine was adopted to carry out the cyclic tests. The adopted strain rates are 0.2% s\(^{-1}\) and 0.4% s\(^{-1}\) in the uniaxial tension and symmetrical strain-controlled cyclic tests, respectively; while the stress rate in the asymmetrical stress-controlled cyclic tests is set to be 200 MPa s\(^{-1}\). The strain data were collected using an extensometer (gage length of 10 mm) in all the macroscopic experiments. The corresponding experimental results are all exhibited in section 3.3, and not discussed here.

3.2. Material parameters

The material parameters employed in this constitutive model can be divided into three categories: (1) The basic mechanical performance parameters, such as elastic modulus \( E \) and Poisson’s ratio \( \nu \), can be directly acquired from the macroscopic experiments. The Burgers vector \( b \) of 6061 aluminum alloy single crystal can be referred to

| Mg | Si | Fe | Cu | Mn | Cr | Zn | Ti | Al |
|----|----|----|----|----|----|----|----|----|
| 0.8–12 | 0.4–0.8 | 0.7 | 0.15–0.4 | 0.15 | 0.04–0.35 | 0.25 | 0.15 | remained |
3.3. Predictions for 6061 aluminum alloy polycrystalline aggregate

Figure 1 provides the uniaxial tensile curves of polycrystalline 6061 aluminum alloy at a strain rate of 0.2% s\(^{-1}\). The model proposed can simulate the uniaxial tensile behavior of 6061 aluminum polycrystalline aggregate precisely. What needs illustration is that the monotonic tensile experimental data were used to determine some of the material parameters by trial-and-error method. Consequently, it is expected that the simulation results have a very high matching with the experimental ones.

With strain rate of 0.2% s\(^{-1}\), the experimental and simulated cyclic stress-strain responses of polycrystalline 6061 aluminum alloy during uniaxial strain cycling are given in figure 2. The mild cyclic hardening characteristic under two strain amplitude can be felicitous described (figure 2(a)), and the evolution of responding stress amplitude can also be captured by this model (figure 2). Despite this, the simulated stress-strain curves do not match the experimental ones perfectly when the hysteresis loop enter into the yielding stage (figure 2(a)). The difference may result from: (1) The revised Armstrong-Frederick nonlinear kinematic hardening adopted in this work only contains one term, rather than more terms type of the more complicate models [36, 37]. Therefore, the stress-strain hysteresis loop can not be simulated precisely. (2) The explicit scale transition rule can not be entirely reflect inter-granular hardening occurred during cyclic loading. In the future work, self-consistent model or generalized scale transition rule should be implanted into the proposed model to improve the simulation of the hysteresis loop.

Finally, the uniaxial ratcheting behavior of 6061 aluminum polycrystalline aggregate under asymmetrical stress cycling is predicted by this model. The uniaxial ratcheting strain \(\varepsilon_r\) is defined as the average value of the peak strain \(\varepsilon_{\text{max}}\) and volley strain \(\varepsilon_{\text{min}}\) in each cycle:

\[
\varepsilon_r = \frac{\varepsilon_{\text{max}} + \varepsilon_{\text{min}}}{2}
\]
The increment of uniaxial ratcheting after each cycle is defined as ratcheting rate, which can be denoted as 
\[ \frac{d\varepsilon_r}{dN} \]. Need not point out that all the stress-controlled cyclic tests involved in this work are all controlled by true stresses. Figure 3 shows the partial hysteresis curves with loading case of 50 ± 320 MPa. Due to the cyclic hardening feature, the hysteresis loops become narrow gradually as the increase of cyclic numbers. The results of uniaxial ratcheting strain versus cyclic numbers with various loading cases are shown in figure 4. Special notes that only the experimental data under loading case of 50 ± 320 MPa were employed to estimate the corresponding material parameters. The uniaxial ratcheting behavior of 6061 aluminum polycrystalline aggregate can be reasonably predicted by this model, which can accurately describe the influence of mean stress and stress amplitude on uniaxial ratcheting strain evolution. Under the same peak stress of 370 MPa, the ratcheting strain rate declines with the increase of stress ratio, as illustrated in figure 4(c).

Figure 5 shows the results of the evolution of ratcheting strain rate versus cyclic numbers under the loading case of 50 ± 320 MPa. The ratcheting strain rate decreases as the cyclic number increases, and finally keeps at a very small constant. The evolution of ratcheting rate can also be captured by the proposed model.

### 3.4. Predictions in intra-granular scale

The model proposed in this paper is constructed in intra-granular scale and expanded to metal polycrystalline using an explicit scale transition rule. Therefore, it is necessary to discuss the capability of this model to predict ratcheting behavior in intra-granular scale. Figure 6(a) shows the predicted results of the ratcheting behavior of 6061 aluminum alloy single crystal in various crystal orientations with a uniform loading case of 50 ± 320 MPa. The ratcheting behavior of the material obviously depends on the crystallographic orientation. Since the weak latent hardening in the single slip orientation, the ratcheting strain rate of the single-slip orientation (−123) is
significantly higher than that of the multiple-slip orientations such as $\{111\}$ and $\{\overline{1}11\}$. This model can also reasonably predict the stress level dependence of single crystal ratcheting deformation, i.e., ratcheting strain and its rate increase with the increase of stress amplitude (figure 6(b)) and mean stress (figure 6(c)). However, due to the lack of relevant experimental data for 6061 aluminum alloy single crystal, only a qualitative prediction and discussion on the crystallographic orientation and stress level dependence of uniaxial ratcheting behavior are illustrated here.

In summary, the proposed model can reasonably simulate the cyclic hardening characteristics of the material. Moreover, the capability of the proposed model to predict the uniaxial ratcheting of polycrystalline...
6061 aluminum alloy has been greatly improved by introducing a revised Armstrong-Frederic kinematic hardening rule associated with cumulative slip. However, the model cannot yet simulate the stress-strain curves well due to the simplified kinematic hardening model and explicit scale transition rule. The proposed model can be improved in the future work by using more complicated kinematic hardening rule and self-consistent model proposed by Hill [31]. Furthermore, some parameters are estimated using trial-and-error method due to absence of corresponding experimental results of 6061 aluminum alloy single crystals, as mentioned in section 3.2. Therefore, systematical experimental researches on single crystals to enhance the predictive ability of the model are urgently needed.

4. Conclusion

Based on the theory of crystal plasticity, a new cyclic ratcheting constitutive model is proposed in intra-granular scale by introducing a revised Armstrong-Frederic kinematic hardening rule associated with cumulative slip and a classical isotropic hardening rule governed by dislocation density. The newly developed model can not only simulate the cyclic hardening characteristics of Polycrystalline 6061 aluminum alloy under symmetric strain-controlled tests, but also the ratcheting behavior under various stress levels. Meanwhile, the proposed model can reasonably simulate the ratcheting behavior under various crystal orientations and stress levels.

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