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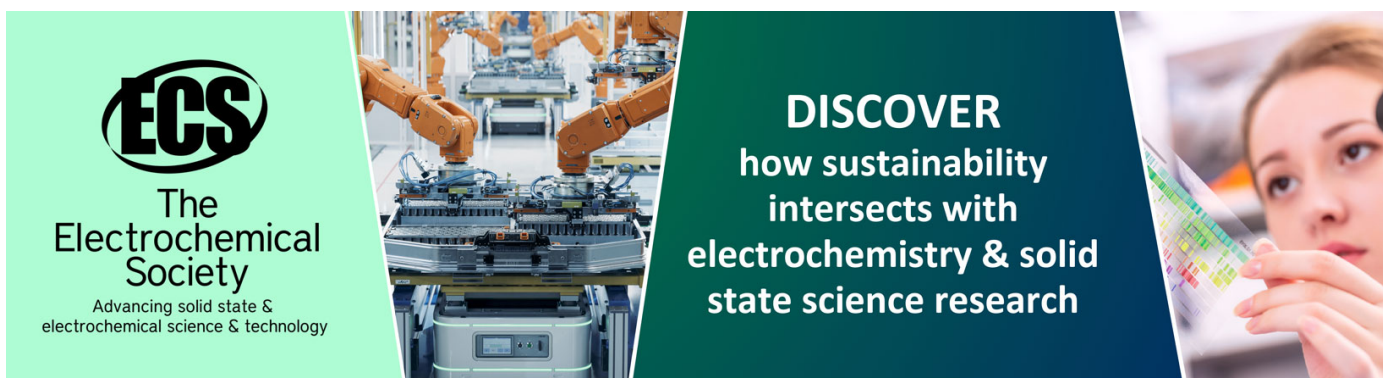
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Crystal Plasticity Modelling of Large Strain Behaviour of HCP Materials

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Abstract. In this paper, we first introduce various polycrystal plasticity models including the Visco-Plastic Self-Consistent (VPSC) model, the Elastic-Plastic Self-Consistent (EPSC) model, and the Elastic Visco-Plastic Self-Consistent (EVPSC) model, as well as twinning models including the Predominant Twin Reorientation (PTR) model and the Twinning and De-Twinning (TDT) model, with emphasizing on characteristic differences between these models. Then, we demonstrate that the EVPSC-TDT model is able to capture key features of large strain behaviour of HCP materials under various deformation processes including uniaxial tension and compression, simple shear, and torsion.

1. Introduction

It has been generally accepted that plastic deformation in most Face Centered Cubic (FCC) and Body Centered Cubic (BCC) crystals is dominated by crystallographic slip, while both slip and twinning contribute to plastic deformation in Hexagonal Close Packed (HCP) crystals. Furthermore, constitutive modeling of twinning is much more difficult than modeling of slip. This is due to the fact that while slip is a gradual process, twinning is a sudden event which causes a dramatic lattice reorientation. Therefore, the first challenging in modeling HCP materials is how to efficiently and accurately account for contribution of twinning to plastic deformation.

Another challenging in constitutive modeling of plastic deformation of HCP materials is due to low crystallographic symmetry and high anisotropy in the mechanical behavior of individual grains. Therefore, at polycrystal level, one must carefully take into account the details of the interaction between grains, because the effects of these details are much more significant than in FCC and BCC materials.

In the present paper, we very briefly review various twinning models including the Predominant Twin Reorientation (PTR) model and the Twinning and De-Twinning (TDT) model, as well as polycrystal plasticity models including the Visco-Plastic Self-Consistent (VPSC) model, the Elastic-Plastic Self-Consistent (EPSC) model, and the Elastic Visco-Plastic Self-Consistent (EVPSC) model, with emphasizing on characteristic differences between these models.



2. Crystal plasticity models and their applications

2.1. Self-consistent polycrystal plasticity models

We start with reviewing crystal plasticity models at polycrystal level. Various polycrystal plasticity models have been developed for polycrystalline materials. Among them, the classic Taylor model (Taylor [1]) has been widely used. The Taylor model assumes that all grains must accommodate the same plastic strain equal to the macroscopically imposed strain. It is well known that the Taylor assumption is reasonable for materials that show a mildly anisotropic plastic response and which are comprised of crystals with many slip systems of comparable strength. Consequently, the Taylor model works quite well for FCC and BCC materials having high crystallographic symmetries. However, the use of the Taylor model for HCP materials may lead to predictions of excessively high stresses, incorrect texture evolutions, or both (Lebensohn et al. [2]). MacEwen et al. [3] have shown that the Taylor-type approach does not work well for the prediction of residual grain-interaction stresses in zirconium alloys. Muransky et al. [4] have demonstrated that the evolution of internal strains and stresses in HCP polycrystalline AZ31 can be predicted based on elastic-plastic self-consistent models. A self-consistent approach appears to be more suitable than the full constraint Taylor approach for constitutive modelling of HCP polycrystals.

The viscoplastic self-consistent (VPSC) model, proposed by Molinari et al. [5] and Lebensohn and Tomé [6], has been successfully applied to simulate large strain behaviour and texture evolution of HCP polycrystalline Mg under various deformations (Agnew and Duygulu [7]). However, the VPSC model does not include elastic deformation and thus cannot be used to study the evolution of lattice strains, which can be used as a very sensitive indicator of plastic deformation mechanisms at microscopic levels. Most of the experimentally measured lattice strain data have been interpreted by using the elastic-plastic self-consistent (EPSC) model developed by Turner and Tomé [8]. However, the EPSC model works only for small deformation and does not include texture evolution associated with slip or twinning reorientation. The EPSC model was extended by Clausen et al. [9] through including texture development and stress relaxation due to twinning. Neil et al. [10] developed a large strain EPSC model to approximately account for the kinematics of large strain, rigid body rotations, texture evolution and grain shape evolution. However, the rate-insensitive character of the constitutive law upon which the EPSC is based, prevents us from addressing strain rate-sensitivity in general, and the experimentally observed stress relaxation and creep associated with finite hold times for data acquisition in particular. It is expected that such a macroscopic relaxation and creep can only be accounted by a rate-sensitive elastic-plastic model. Mareau and Daymond [11] developed an elasto-viscoplastic self-consistent (EVPSC) model to describe the behaviour of HCP materials where multiple deformation modes, including plastic slip and twinning, coexist. The model was applied to study the development of lattice strains in a moderately textured Zircaloy-2 slab. However, the EVPSC model by Mareau and Daymond [11] works only for small deformations, and relaxation during individual measurements was not explicitly accounted for in their simulations.

A finite strain elastic-viscoplastic self-consistent (EVPSC) model for polycrystalline materials has been developed by Wang et al. [12]. This EVPSC model is a completely general elastic-viscoplastic, fully anisotropic, self-consistent polycrystal model, applicable at large strains and to any crystal symmetry. They have shown that at large monotonic strains elasticity saturates and the EVPSC model gives results very close to the very popular VPSC model. For deformations involving elasto-plastic transients associated with unloading and strain path changes, the EVPSC predicts clear and gradual transitions, while VPSC gives stress discontinuities due to the lack of elastic deformation. It has been also demonstrated that the EVPSC model can capture some important experimental features which cannot be simulated using the VPSC model.

Wang et al. [12] have found that numerical results based on the VPSC and EVPSC models are extremely sensitive to the stiffness of the grain-matrix interaction associated with the various self-consistent schemes (SCSs) including the Secant, Affine, Tangent and the effective interaction meff. Various self-consistent schemes used in self-consistent modelling have been evaluated. It has been

demonstrated that the Affine self-consistent scheme gives the best overall performance among the self-consistent approaches examined for magnesium alloy AZ31B (Wang et al. [13]), Zr alloys (Qiao et al. [14]), and even for FCC materials such as stainless steel (Guo et al. [15]) and OFHC copper (Guo et al. [16]).

2.2. Twinning models

We proceed by reviewing the available twinning models used in the VPSC, EPSC and EVPSC models. Most of the current available twinning models, including the Predominant Twin Reorientation (PTR) scheme proposed by Van Houtte [17], Tomé et al. [18] and Lebensohn and Tomé [6] and later extended by Clausen et al. [9], and the twinning scheme developed by Kalidindi [19], have been developed mainly to describe the reorientation due to twinning and hardening evolution associated with twinning. However, they are not able to describe detwinning because they do not specifically address detwinning. The composite grain (CG) model proposed by Proust et al. [20] is exception, which is aiming for both twinning and detwinning and can be implemented in a polycrystal plasticity model. However, the CG model contains many mechanisms and features that are difficult to be characterized. In addition, the highly empirical way of treating twin nucleation and twin propagation stresses employed in the CG model has been superseded by the nucleation model developed by Beyerlein et al. [21].

The Twinning and De-Twinning (TDT) model developed by Wang et al. [22, 23] assumes that a grain has four potential operations associated with twinning and detwinning. As shown in Fig. 1, Operation A is twin nucleation and initiates a twin band or 'child'. Operation B is a propagation of the child into the parent grain. Operations A and B increase the twin volume fraction and thus correspond to twinning. Operation C is a propagation of the parent into the child. Operation D splits the twin band and decreases the twin volume fraction through re-twinning. Operations C and D decrease the twin volume fraction and thus correspond to detwinning.

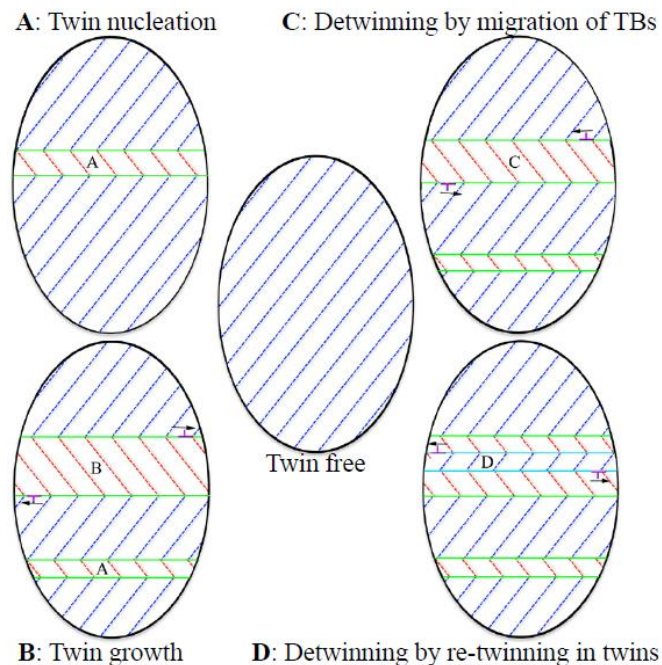


Figure 1. Schematic representation of twinning and detwinning in a grain.

Because it is rare that a grain can be fully twinned, a threshold twin volume fraction is defined in the model to terminate twinning. Consequently, both the PTR model and the TDT model introduce two statistical variables: accumulated twin fraction, v^{acc} , and effective twinned fraction, v^{eff} . More

specifically, V^{acc} and V^{eff} are the weighted volume fraction of the twinned region and volume fraction of twin terminated grains, respectively. The threshold volume fraction, V^{th} , is defined as $V^{th} = \min\left(1.0, A_1 + A_2 \frac{V^{eff}}{V^{acc}}\right)$, where A_1 and A_2 are two material constants.

An advantage of the PTR approach is that it is computationally efficient. There is no increase in the number of grains that must be tracked by the code. However, there are two disadvantages that may become significant if strain path changes are of interest, especially at small or intermediate strain levels. The first is the fact that the volume fraction of reoriented material V^{eff} does not at all points properly correlate with the amount of twinning which has taken place V^{acc} (though it does match at higher strain levels). The second aspect is that not every activated twin variant is present in the final simulated “microstructure,” since only the predominant twin variant is respected by the model. This may be fine for cases in which a single twin variant dominates. However, there may be cases when many variants are observed to occur.

The TDT model considers a twin as a new grain in the sense that a new ellipsoid is added to the 1-site self-consistent formulation. The orientation of the new grain is initially related to that of the parent through the crystallographic twin relation, which reorients the c-axis by 86.3° . However, it is worth mentioning that twin only “interacts” with its parent through the self-consistent equations during subsequent straining steps. These equations enforce the same critical shear stresses for twinning and govern the exchange of volume fraction between the twin and its parent. In short, there is no special enforcement equilibrium or compatibility between the twin and parent. Rather, the twin and parent are forced to satisfy equilibrium and compatibility with the homogeneous equivalent medium (HEM). It is important to mention that the TDT model does not introduce any additional parameters for detwinning. The simulated detwinning process is a natural outcome of the proposed TDT model.

Very recently, a new empirical equation for describing the termination of twinning in magnesium alloys was developed by Qiao et al. [24]. The new description introduces only a single parameter. It has been demonstrated that it is easy to calibrate the single parameter and the proposed empirical equation is able to capture key macroscopic features associated with twinning and its termination experimentally observed in a variety of magnesium alloys with different textures, including a nearly randomly textured casting.

Based on the TDT model, Wu et al. [25] have developed a new twin nucleation, propagation and growth (TNPG) model for HCP materials. The TNPG model explicitly takes into account the stress relaxation associated with twin initiation and propagation. It has been rationalized that the stress relaxation drives a just nucleated twin to propagate, while work-hardening makes the twin grow after its propagation. It has been demonstrated that the new twinning model is able to capture key macroscopic features associated with twin nucleation and propagation experimentally observed in the wrought magnesium alloys.

It is worth mentioning that Qiao et al. [26] have recently extended the TDT model to allow studying secondary/double twinning. The deformation characteristics of rolled Mg alloy AZ31, which was previously compressed along the rolling direction and then re-compressed along the transverse direction, have been numerically investigated. $\{10\text{-}12\}$ - $\{10\text{-}12\}$ secondary twinning is found to play an important role in reproducing the experimental data.

Finally, it is interesting to note that Agnew et al. [27] very recently used different values of material parameters describe hardening for materials in twinned and untwined areas. This modification of the TDT model has the advantage of being able to describe the internal strains within twins in addition to the flow stress and texture evolution.

2.3. Applications of the EVPSC and TDT models

The EVPSC model has been used to study the lattice strain evolution in extruded magnesium alloy AZ31 under uniaxial tension and compression. The results have been compared against in-situ neutron diffraction measurements done on the same alloy. For the first time, the effects of stress relaxation and

strain creep on lattice strain measurements in respectively displacement controlled and load controlled in-situ tests were numerically assessed. It has been found that the stress relaxation has a significant effect on the lattice strain measurements. It has been also observed that although the creep does not significantly affect the trend of the lattice strain evolution, a better agreement with the experiments is found if creep is included in the simulations (Wang et al. [28]).

The effect of stress relaxation and creep on lattice strain evolution of stainless steel under tension has been also experimentally and numerically studied (Wang et al. [29]). In this work, an in-situ neutron diffraction technique, which consists in performing the diffraction measurements using continuous event-mode data collection while conducting the mechanical loading monotonically with a very slow loading rate, was proposed to avoid the effects associated with interrupts. The lattice strains in stainless steel under uniaxial tension were measured using the three techniques: the two main experimental approaches rely on loading the specimen at a rate of typically $\sim 10^{-4}$ - 10^{-3} /s and periodically interrupt the test and hold either the macroscopic strain or the macroscopic stress constant during data collection, and the third one is with a very slow loading rate ($\sim 10^{-6}$ /s) while collecting data continuously. The experimental results were compared to study the effect of stress relaxation and strain creep on the lattice strain measurements. The experimental results were simulated using both the EVPSC and EPSC models. It was found that both the EVPSC and EPSC models give reasonable predictions for all the three tests, with EVPSC having the added advantage over EPSC that it allows us to address the relaxation and creep effects in the interrupted tests. It has been emphasized that a single set of EVPSC hardening parameters can address monotonic, relaxation and creep results of internal strain and macroscopic stress-strain evolution. By comparison, the EPSC approach, which does not account for viscous response, can well reproduce the results only if different sets of hardening parameters are used to simulate the relaxation, creep or monotonic tests. The fact that the EPSC parameters are 'test dependent' and that it is not possible to simulate relaxation or creep, points at a limitation of the EPSC model. It has been concluded that the EVPSC is better suited to interpret neutron diffraction of moderate to very rate sensitive materials, than the rate-insensitive EPSC model.

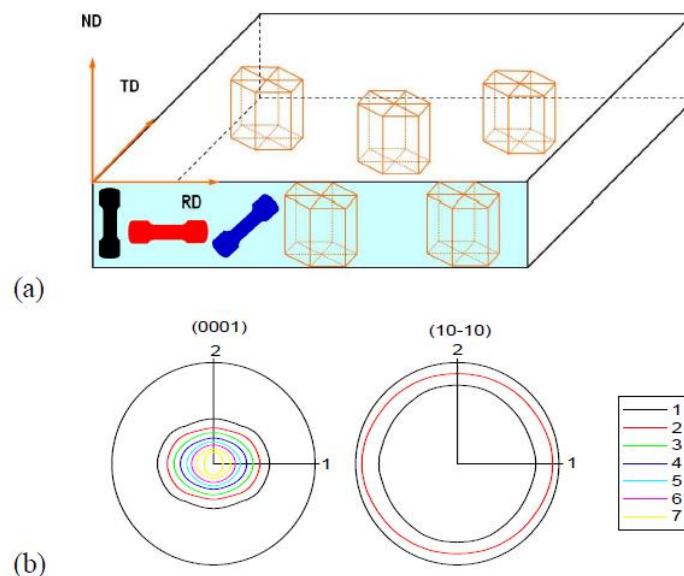


Figure 2. (a) Schematic representation of testing samples along the RD, ND and 45° with respect to the RD in the RD-ND plane; (b) initial texture in terms of the $\{0001\}$ and $\{10-10\}$ pole figures.

The TDT model has been implemented into the EVPSC framework. The EVPSC-TDT model has been applied to study the large strain behavior of Mg alloys under various deformation processes. Fig. 2 presents a schematic representation of testing samples along the rolling direction (RD), normal

direction (ND), and 45° with respect to the RD in the RD-ND plane for a rolled thick plate AZ31B. Also included in Fig. 2 is the initial texture in terms of the $\{0001\}$ and $\{10\cdot10\}$ pole figures. Values of the material parameters involved in the EVPSC-TDT model are listed in Table 1

Table 1. List of values of the material parameters involved in the EVPSC-TDT model.

Mode	τ_1 (MPa)	τ_2 (MPa)	h_0 (MPa)	h_1 (MPa)	$h^{\alpha\beta}$	A_1	A_2
Basal	12	1	10	0	1		
Prismatic	78	55	600	35	1		
Pyramidal	100	140	3000	50	1		
Extension twin	35	0	0	0	1	0.65	0.75
Compressive twin	185	0	0	0	1	0.65	0.75

Figures 3-5 show the measured and simulated monotonic uniaxial tension and compression stress and strain curves along the RD (Fig. 3), ND (Fig. 4) and 45° (Fig. 5).

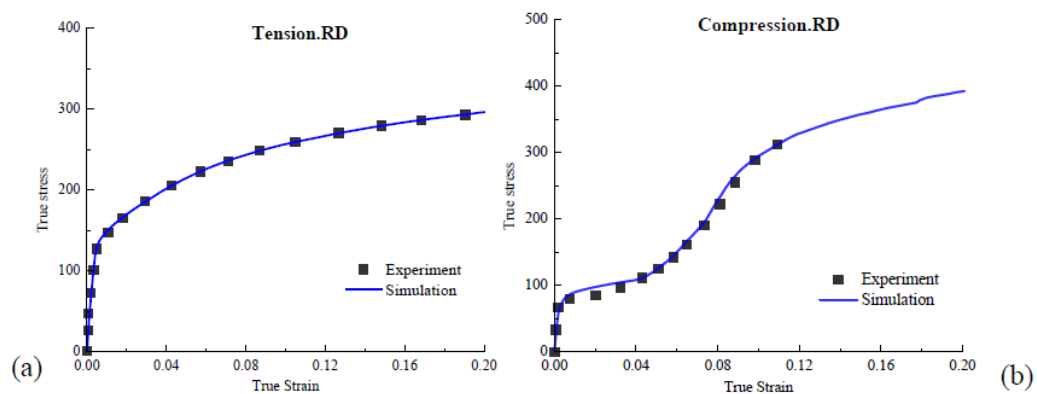


Figure 3. The measured and simulated stress-strain curves under uniaxial tension (a) and compression (b) along the RD.

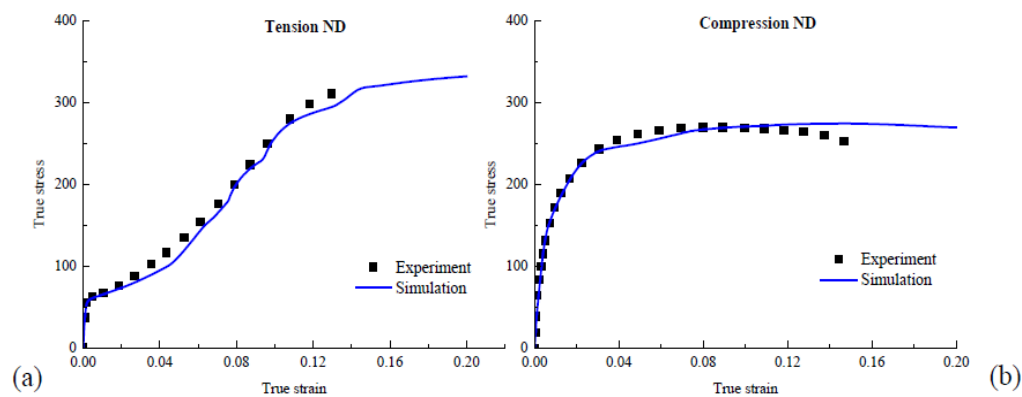


Figure 4. The measured and simulated stress-strain curves under uniaxial tension (a) and compression (b) along the ND.

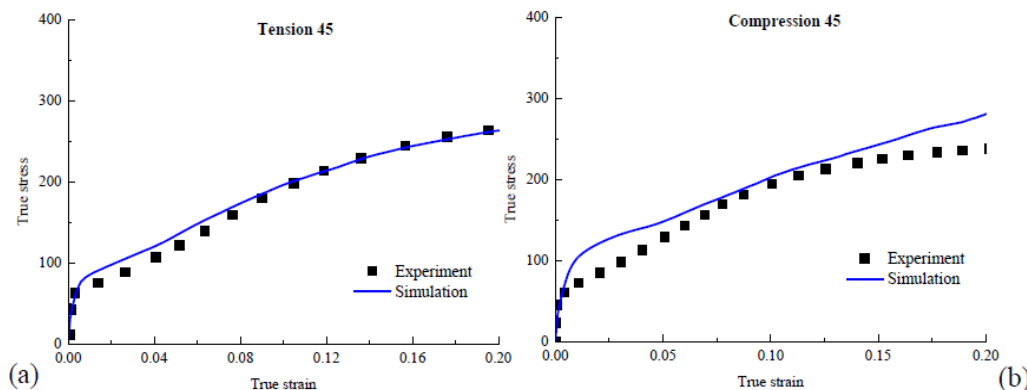


Figure 5. The measured and simulated stress-strain curves under uniaxial tension (a) and compression (b) along 45° with respect to the RD.

Results shown in Figs. 3-5 demonstrate that a single set of EVPSC-TDT hardening parameters permits prediction of the strength anisotropy and monotonic strain hardening behavior along any tilt angle with respect to the RD.

It has been noticed that most of the research has been restricted to tension and compression along different directions, where the principal stresses/strains do not change their directions during the deformation processes. This kind of study implies that some important mechanical behavior associated with shear might not be revealed by only studying these tension and compression deformation processes. Guo et al. [30] have experimentally and numerically studied a rolled AZ31B thick plate with a strong basal texture under free-end torsion. It has been demonstrated that the Swift effect in the material under free-end torsion is mainly due to extension twinning.

It is worth mentioning that the predicative capability of the EVPSC-TDT model can be more efficiently demonstrated by applying it to simulate deformation processes involving cyclic loadings and strain path changes. For example, lattice strain evolutions under cyclic loadings were successfully investigated by Wu et al. [31] for rolled AZ31 plate and by Qiao et al. [32] for extruded ZK60 plate.

3. Conclusions

It has been demonstrated that the EVPSC-TDT model is able to capture key features associated with twinning and detwinning observed experimentally. However, it is important to point out that the TDT model in its current form can be considered, to some extent, as a purely geometrical twinning-detwinning model in the sense that, although the present TDT model rigorously calculates the shear rates, twin volume fraction and reorientation due to twinning and detwinning, it does not directly account for effects of twinning on hardening associated with dislocation slips. It is expected that the new twinning model's predictive capability could be further enhanced once interaction between twinning and slip is considered. This work is in progress and will be reported elsewhere.

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