Microstructures

Supplementary Materials

A mechanics-informed deep learning constitutive model for sequential prediction of strain rate-dependent behavior and microstructural evolution

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Supplementary Material 1. Detailed implementation of the polycrystalline constitutive model EVPSC

This appendix provides a detailed implementation of the dataset generator, the polycrystalline constitutive model EVPSC, introduced in section 3.1. The model integrates dislocation and twinning mechanisms, using a dislocation velocity model across a wide range of strain rates and the twinning model. A self-consistent framework[1,2] is employed to simulate the polycrystalline system, incorporating grain boundary-related dislocation evolution. The impact of grain boundaries on strain-rate sensitivity is also incorporated in this model. For clarity and ease of reference, the calibrated model parameters and the notations used in the following equations are summarized in Tables S1 and S2, respectively.

The polycrystalline constitutive relation is expressed in a pseudo-linear form, consisting of an elasticity term, which relates the Jaumann rate of the Cauchy stress, and plasticity terms, as follows[3,4]:

$$D_{ij} = \bar{M}^{e}_{ijkl}\dot{\Sigma}^{\nabla}_{kl} + \bar{M}^{p}_{ijkl}\Sigma_{kl} + D^{0}_{ij} \tag{S.1}$$

For each single crystal, a similar relationship holds[5]:

$$d_{ij} = M^{e,g}_{ijkl}\dot{\sigma}^{\nabla}_{kl} + M^{p,g}_{ijkl}\sigma_{kl} + d^{0}_{ij} \tag{S.2}$$

The monocrystal response is obtained through the localization relation from the macroscopic polycrystal response, using the localization factors B^{g}_{ijkl} and b^{g}_{ij}[5]:

$$\sigma_{ij} = B^{g}_{ijkl}\Sigma_{kl} + b^{g}_{ij} \tag{S.3}$$

In each grain, the plastic deformation is the sum of dislocation-induced and twinning-induced plasticity[5]:

$$d^{p}_{ij} = d^{dis}_{ij} + d^{tw}_{ij} \tag{S.4}$$

The dislocation-induced plasticity is calculated by summing shear strain rate tensors across all related slip systems[6]:

$$d^{dis}_{ij} = \sum_{\alpha=1}^{n} s^{\alpha}_{i} n^{\alpha}_{j} \dot{\gamma}^{\alpha} = \sum_{\alpha=1}^{n} s^{\alpha}_{i} n^{\alpha}_{j} \rho^{\alpha} b^{\alpha} v^{\alpha} \tag{S.5}$$

For twinning-induced plasticity, similar equation is also adopted[2]:

$$d_{ij}^{tw} = \sum_{\alpha=1}^{n} s_i^{\alpha} n_j^{\alpha} \dot{\gamma}_{tw}^{\alpha} \quad (S.6)$$

The control equations governing dislocation behavior will primarily focus on a single-slip system. In this case, the notation for the slip system, α, will be omitted. The resistance to dislocation movement is modeled as a combination of dislocation forest hardening, the Hall-Petch effect, and the accumulation of dislocations at grain boundaries[7-11]:

$$\tau_r = c_h G b \sqrt{\sum_{\beta}^{N} h^{\alpha\beta} \rho^{\beta}} + c_h h_{GB} G \sqrt{b/\pi \bar{D}} + c_h G b \sqrt{\rho_{acc}} \quad (S.7)$$

where $h^{\alpha\beta}$ is determined from different dislocation interaction/junction types as $h_{NJ}, h_{HL}, h_{CJ}, h_{GJ}$ and h_{SJ} [2][10]. With this resistance, the dislocation movement follows a three-regime law, which includes thermal activation, phonon drag, and velocity saturation[12-14]:

$$v = \bar{L}/(t_w + t_r) \quad (S.8)$$

$$t_w = \frac{1}{\mathrm{v}_0} \exp\left(\frac{Q_0}{k_B T}\left[1 - \mathrm{sgn}(|\tau| - \tau_r)\left(\frac{\left||\tau| - \tau_r\right|}{\tau_c}\right)^{\xi}\right]\right) \quad (S.9)$$

$$t_r = \frac{\bar{L}}{v_s\left(\sqrt{1 + \left(\frac{v_s}{2\widehat{v_r}}\right)^2} - \frac{v_s}{2\widehat{v_r}}\right)} \quad (S.10)$$

$$\widehat{v_r} = \frac{b}{B_0}(|\tau| - \tau_r) \quad (S.11)$$

The evolution of dislocations is governed by processes such as heterogeneous nucleation, multiplication, coplanar reactions, and annihilation recovery, along with the contribution of dislocation nucleation at grain boundaries. These processes are expressed as[12,15,16]:

$$\frac{d\rho}{d\gamma}=\frac{d\rho_{nuc}}{d\gamma}+\frac{d\rho_{nuc,s}}{d\gamma}+\frac{d\rho_{mul}}{d\gamma}+\frac{d\rho_{copl}}{d\gamma}-\frac{d\rho_{ann}}{d\gamma} \tag{S.12}$$

The heterogeneous nucleation and grain boundary nucleation terms share a similar form [2,17]:

$$\frac{d\rho_{nuc}}{d\gamma}=k_{\rho,nuc}\frac{\left|\tau-\tau_{c,nuc}\right|}{Gb^2} \tag{S.13}$$

$$\frac{d\rho_{nuc,s}}{d\gamma}=k_s\frac{\pi\overline{D}^2 b}{V_s}\frac{\left|\tau-\tau_{nuc,s}\right|}{Gb^2} \tag{S.14}$$

where V_s is the activation volume of the grain boundary nucleation, and is set as $100b^3$ The multiplication and annihilation recovery terms are presented as[2,14]:

$$\frac{d\rho_{mul}}{d\gamma}=\frac{k_{\rho,mul}}{\overline{L}} \tag{S.15}$$

$$\frac{d\rho_{ann}}{d\gamma}=\left(\frac{d\rho_{nuc}}{d\gamma}+\frac{d\rho_{mul}}{d\gamma}\right)\left[\frac{c_h b}{g}\left(1-\frac{k_B T}{Db^3}\log\frac{|\dot{\varepsilon}|}{\dot{\varepsilon}_0}\right)\right]^2\rho \tag{S.16}$$

The coplanar reaction describes the evolution of the coplanar slip system. In FCC {111}<110> slip systems, three coplanar slip systems share a single slip plane. For slip system γ and its coplanar systems α and β, this relationship is expressed as[18]:

$$\begin{aligned}\dot{\rho}^{\gamma}_{copl} = {} & \dot{\rho}^{\gamma,\alpha\beta}_{copl}-\dot{\rho}^{\alpha,\beta\gamma}_{copl}-\dot{\rho}^{\beta,\alpha\gamma}_{copl}\\ = {} & c_{copl}\left[\left(\sqrt{\rho^{\beta}}\rho^{\alpha}v^{\alpha}+\sqrt{\rho^{\alpha}}\rho^{\beta}v^{\beta}\right)-\right.\\ & \left.\left(\sqrt{\rho^{\gamma}}\rho^{\beta}v^{\beta}+\sqrt{\rho^{\beta}}\rho^{\gamma}v^{\gamma}\right)-\left(\sqrt{\rho^{\alpha}}\rho^{\gamma}v^{\gamma}+\sqrt{\rho^{\gamma}}\rho^{\alpha}v^{\alpha}\right)\right]\end{aligned} \tag{S.17}$$

Dislocation accumulation at grain boundaries is modeled as:

$$\frac{d\rho_{acc}}{d\gamma} = \sqrt{\frac{l'}{\bar{D}}}\frac{d\rho_{ann}}{d\gamma} \quad (S.18)$$

where l' is the characteristic length for dislocation interaction with grain boundary, set to 11b here[19,20].

For twinning mechanisms, only twin nucleation and growth are considered. The shear strain rate and the twin volume fraction change rate for the twin system α are given by:

$$\dot{\gamma}_{\mathrm{tw}}^{\alpha} = \begin{cases} \dot{\gamma}_0^{\alpha}|\tau^{\alpha}/\tau_{cr}^{\alpha}|^{1/m} & \tau^{\alpha} > 0 \\ 0 & \tau^{\alpha} \leq 0 \end{cases} \quad (S.19)$$

$$\dot{f}_{\mathrm{tw}}^{\alpha} = (f^M + f^{\alpha})|\dot{\gamma}_{\mathrm{tw}}^{\alpha}|/\gamma^{tw} \quad (S.20)$$

where $\gamma^{tw} = 0.471$ is the reference shear strain for FCC {111}<112> twinning [19][21]. To regulate twin expansion, the critical twin volume fraction V_{th} is defined as:

$$V_{th} = \min\left(1.0, A_1 + A_2\frac{V_{eff}}{V_{acc}}\right) \quad (S.21)$$

The model parameters were determined by calibration from the experimental stress strain curves at strain rates of 0.001/s and 3000/s. The calibrated model was then validated by reproduce the stress responses in other four strain rates listed in Figure 4. The calculated dislocation density extents as well as the twin volume fractions are all consistent to the experimental observations, verified the capability of this EVPSC model in capturing the complex strain rate sensitive behavior. The model parameters are given in Table S1.

Table S1. EVPSC model parameters describing the CrFeNi polycrystalline system

Parameter	Value	Parameter	Value
Dislocation Movement			
ν_0	1010 /s	Q_0	0.92 eV

τ_c	200 MPa	ξ	0.8
v_s	1500 m/s	c_d	6
Dislocation Evolution			
$k_{\rho,nuc}$	0.2	$\tau_{c,nuc}$	120 MPa
k_s	0.0031	$\tau_{nuc,s}$	380 MPa
$k_{\rho,mul}$	6×108 /m	$\dot{\varepsilon}_0$	3×108 /s
D	800 MPa	g	0.0025
c_{copl}	0.16		
Dislocation Interaction			
c_h	0.1	h_{NJ}	1
h_{HL}, h_{CJ}	1.5	h_{GJ}, h_{SJ}	2.2
h_{GB}	1.3		
Twinning			
$\dot{\gamma}_0$	3000 /s	m	0.007
τ_{cr}	380 MPa	A1	0.1
A2	0.8		

Table S2. Nomenclature of symbols used in the polycrystalline crystal plasticity model

Symbol	Definition	Unit
D	The polycrystalline stretching tensor	s^{-1}
$\bar{M}^e$	The polycrystalline elastic compliance tensor	MPa^{-1}
$\bar{M}^p$	The polycrystalline visco-plastic compliance tensor	MPa^{-1}
Σ	The polycrystalline stress tensor	MPa
$\dot{\Sigma}^\nabla$	Jaumann rate of the polycrystalline stress tensor	MPa/s
D^0	Linear extrapolate term of the polycrystalline stretching tensor	s^{-1}
d	The monocrystalline stretching tensor	s^{-1}
$M^{e,g}$	The monocrystalline elastic compliance tensor	MPa^{-1}
$M^{p,g}$	The monocrystalline visco-plastic compliance tensor	MPa^{-1}
σ	The monocrystalline stress tensor	MPa
$\dot{\sigma}^\nabla$	Jaumann rate of the monocrystalline stress tensor	MPa/s

d^0	Linear extrapolate term of the monocrystalline stretching tensor	s^{-1}
B^g	Localization factor from polycrystal stress to monocrystal stress	--
b^g	Linear extrapolate term in the localization relationship	MPa
d^p	The monocrystalline visco-plastic stretching tensor	s^{-1}
d^{dis}	The monocrystalline stretching tensor contributed by dislocation	s^{-1}
d^{tw}	The monocrystalline stretching tensor contributed by twinning	s^{-1}
s^α	Slip direction vector / Twinning shear direction vector	--
n^α	Slip plane normal vector / Twin boundary normal vector	--
$\dot{\gamma}^\alpha, \dot{\gamma}^\alpha_{tw}$	Shear strain rate of a slip system / twin system	s^{-1}
ρ^α, ρ	Dislocation density of a slip system	m^{-2}
b^α, b	Burgers vector length of a slip system	m
v^α, v	Dislocation velocity of a slip system	m/s
G	Shear modulus of a slip system	MPa
τ_r	Slip resistance of a slip system	MPa
c_h	Dislocation hardening parameter	--
$h^{\alpha\beta}$	Dislocation interaction factor between slip system α and β	--
$h_{NJ}, h_{HL}, h_{CJ}, h_{GJ}, h_{SJ}$	Interaction factor for no junction, Hirth Lock, coplanar junction, glissile junction and sessile junction	--
h_{GB}	Dislocation-grain boundary interaction factor	--
$\overline{D}$	Average grain size (diameter)	m
ρ_{acc}	Accumulated dislocation density on grain boundaries.	m^{-2}
$\overline{L}$	Mean free path in a single crystal	m
t_w	Waiting time of dislocation movement	s
t_r	Running time of dislocation movement	s
ν_0	Reference frequency of the thermal activation process	s^{-1}
Q_0	Activation energy of the thermal activation process	eV
k_B	Boltzmann constant	J/K
T	Temperature of the polycrystalline system	K
τ	Resolved shear stress of a slip system	MPa

τ_c	Slip friction stress of a slip system	MPa
v_s	Saturated velocity of a slip system	m/s
B_0	Drag coefficient of dislocation movement	MPa.s
ρ_{nuc}, $\rho_{nuc,s}$, ρ_{mul} , ρ_{copl} , ρ_{ann}	Dislocation density variation attributed by heterogeneous nucleation, grain boundary nucleation, multiplication, coplanar reaction and annhilation/recovery	m^{-2}
$k_{\rho,nuc}$, k_s	Nucleation coefficient for heterogeneous nucleation and grain boundary nucleation	--
V_s	Activation volume of the grain boundary nucleation	m^3
$k_{\rho,mul}$	Dislocation multiplication factor	m^{-1}
D	Drag stress of dislocation	MPa
g	Normalized activation energy of dislocation recovery	--
$\dot{\varepsilon}_0$	Reference strain rate of slip system	s^{-1}
$\dot{\rho}_{copl}^{\gamma,\alpha\beta}$	Dislocation coplanar reaction rate on system γ from systems α and β	m^{-2} s^{-1}
c_{copl}	Dislocation coplanar reaction coefficient	--
l'	Characteristic length for dislocation interaction with grain boundary	m
$\dot{\gamma}_0^{\alpha}$	Reference shear strain rate of twinning	s^{-1}
τ_{cr}^{α}	Critical shear stress of the twinning system	MPa
f^{α}, f^{M}	Volume fraction of a twin variant and the matrix	--
γ^{tw}	Character shear strain of twinning	--
V_{th}	Critical twin volume fraction to regulate twin expansion	--
V_{acc}	Total twin volume fraction in the polycrystal	--
V_{eff}	Volume fraction of the grain under consideration	--
A1, A2	Twin volume fraction controlling parameters	--

Supplementary Material 2. Assessment of Model Generalization and Reproducibility

The 5-fold cross-validation results indicate that the model maintains stable predictive performance across different data splits, with an average MSE of 0.0288 ± 0.0010 and MAE of 0.1016 ± 0.0024, suggesting good generalization ability. The five repeated runs further show that the model is not highly sensitive to random initialization or training stochasticity under the same data split, with an average MSE of 0.0282 ± 0.0005 and MAE of 0.1002 ± 0.0013, demonstrating strong training stability and reproducibility.

To further assess the generalization of MIDLCM across data partitions, a 5-fold cross-validation was conducted at the case level. All 756 cases were divided into five approximately equal folds while preserving representative distributions of strain paths and strain rates. In each round, one fold was used as the test set and the remaining four folds were used for training, following the same training protocol as in the main text, including Xavier initialization, AdamW optimization with cosine annealing, gradient clipping, and validation-loss-based checkpoint selection.

To evaluate the sensitivity of the model to training stochasticity, five repeated experiments were further performed under the original 4:1 case-based train/test split. In these runs, the network architecture, hyperparameters, optimizer settings, and data split were fixed, and only the random initialization and stochastic training process were changed. The corresponding MSE and MAE values are summarized in Table S3, showing only minor fluctuations across runs and therefore confirming the stability and reproducibility of the proposed model.

Table S3. Results of 5-fold cross-validation and five repeated runs with different random initializations

Index (Fold / Run)	**5-fold cross-validation**		**Random initialization repeats**	
	MSE	MAE	MSE	MAE
1	0.0276	0.0990	0.0282	0.1000
2	0.0288	0.1010	0.0279	0.0990
3	0.0301	0.1050	0.0285	0.1010
4	0.0294	0.1030	0.0288	0.1020
5	0.0283	0.1000	0.0276	0.0990
Mean ± SD	0.0288 ± 0.0010	0.1016 ± 0.0024	0.0282 ± 0.0005	0.1002 ± 0.0013

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