



Thermo-micro-mechanical modeling of plasticity and damage in single-phase S700 steel

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ABSTRACT

In this study, a Thermo-micro-mechanical (TMM) model to describe the viscoplastic flow of polycrystalline metallic materials was extended by integration of micromechanical damage. The original TMM model [1] incorporated the fundamentals of dislocation motions during metal deformation, using microstructural state variables (MSVs) for the statistical quantification of dislocations, represented through the dislocation density. These MSVs track dislocation evolution throughout deformation, allowing for the material behavior and mechanical properties in cold and warm regimes (up to 500 °C) to be derived as functions of these state variables. A key advantage of the TMM model is its ability to transfer MSVs across multi-step process chain simulations, thereby accounting for the deformation history of materials in subsequent processes. However, the previous model was limited to the plastic regime and cannot be applied to processes involving damage and fracture. The primary objective of the current study is to extend the TMM model to predict fracture and damage. Therefore, the Gurson-Tveergard-Needleman (GTN) model, a widely recognized micromechanical damage model, was integrated into the TMM model to describe the material behavior comprising plasticity, damage and fracture (D-TMM model). This integration introduces void fraction from the damage model as an additional state variable alongside the existing MSVs, thus enabling the transfer of both deformation history and damage accumulation across the process chain. The constitutive equations from both models are numerically integrated, and their parameters are calibrated for a commonly used micro-alloyed high strength construction steel – S700. The model is subsequently tested under isothermal conditions up to 500 °C, non-isothermal conditions, and across a range of strain rates.

1. Introduction

Finite Element (FE) simulations play a critical role in product and process development by optimizing resource utilization, including manpower and materials, and are widely recognized for their effectiveness in enhancing efficiency and reducing resource consumption, as evidenced by studies such as [2–5]. However, a significant challenge in FE simulations is the accurate representation of material behavior, as different methods are applied to achieve this [6,7]. Traditionally, empirical material models are used to represent plasticity and damage in deformation processes [8,9], though they typically ignore the material's deformation history. This is a critical limitation in multi-step manufacturing processes simulations, where material properties evolve with each deformation step, directly affecting subsequent responses [10,11].

To overcome these limitations, multiscale modeling approaches have emerged, integrating material models that account for microstructural characteristics, including dislocation density, grain size, and phase fractions etc., [12–14]. By incorporating evolution equations for these microstructural features, multiscale models can more precisely capture the material's behavior during deformation. In multi-step manufacturing processes, these models allow the evolved microstructural state from one step to become the starting point for the next step, effectively embedding the material's deformation history within the simulation framework [15]. This integration significantly enhances the predictive accuracy of FE simulations, facilitating more efficient resource use and improving overall product quality by providing a more realistic assessment of material responses across complex manufacturing sequences.

Motaman et al. [1] introduced a thermo-micro-mechanical (TMM) model that uses dislocation density as an internal state variable to

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Nomenclature			
Symbol Description			
$\mathbb{C}$	Fourth order stiffness tensor [Pa]	pw	Plastic stress from wall dislocation
A	Material specific parameter associated to void nucleation [-]	x	Cell, wall or total ($x = c, w, t$)
B	Left Cauchy deformation stress tensor [-]	ν	Viscous
C	Right Cauchy deformation stress tensor [-]	0	Reference/ initial state
C	Hardening capacity [-]	$+$	Increase
D	Rate of deformation tensor [s^{-1}]	$-$	Decrease
E	Elastic modulus [Pa]	cm	Cell mobile
F	Deformation gradient tensor [-]	ci	Cell immobile
G	Shear modulus [Pa]	wi	Wall immobile
J	Jacobian [deformation map]	an	Annihilation
K	Bulk modulus [Pa]	ac	Accumulation
L	Velocity gradient tensor [s^{-1}]	nc	Nucleation
M	Taylor factor [-]	rm	Remobilization
R	Orthogonal rotation tensor [-]	gn	Generation
R	Residual function in Newton-Raphson scheme [-]	tr	Trapping
S	Yield to tensile ratio [-]	z	Process – an, ac, nc, rm, gn, tr
T	Temperature [$^{\circ}C$]	h	Hydrostatic stress
U	Right stretch tensor [-]	y	Yield stress
V	Volume [m^3]	eq	Equivalent stress
V	Left stretch tensor [-]	f_{indx}	Indx – c – critical fraction, f – failure fraction, n – nucleation fraction
W	Spin tensor [s^{-1}]	$nucl$	Void nucleation
b	Burger's length [m]	$growth$	Void growth
f	Void fraction [-]	$trial$	Trial step
l	Length of dislocation segments [m]	(n)	Time increment index
m	Strain rate sensitivity parameter [-]	$(n + 1)$	Current time increment index
n	Yield surface normal tensor [-]	$\{k\}$	Newton-Raphson iteration index
q	Tvergaard constant [-]	$\{k + 1\}$	Current Newton-Raphson iteration step
r	Temperature sensitivity coefficient	Abbreviation Description	
s	Temperature sensitivity exponent [-]	AHSS	Advanced high strength steel
t	Time [s]	ASTM	American society for testing and materials
u	Displacement [m]	CB	Cell block
v	Velocity vector [ms^{-1}]	CDD	Continuum dislocation dynamics
x	Position vector (spatial coordinate) [m]	CMD	Continuum microstructure dynamics
I	Identity tensor [-]	CT	Compact tension (test specimen)
S	Stochastic state set [set of all MSVs]	DSA	Dynamic strain ageing
s	Deviatoric part of the stress tensor [-]	DTH	Dynamic thermal hardening
α	Dislocation interaction coefficient [-]	DTS	Dynamic thermal softening
γ	Shear strain in slip system [-]	EBSD	Electron backscatter diffraction
ε	Mean true strain [-]	FE	Finite element
λ	Consistency or plastic parameter [-]	FEMU	Finite element model updating
ν	Poisson's ratio [-]	GNB	Geometrically necessary boundaries
ρ	Dislocation density [m^{-2}]	GND	Geometrically necessary dislocations
σ	Mean true stress [Pa]	GTN	Gurson-tveergard-needleman
τ	Resolved shear stress [Pa]	HSS	High strength steel
χ	Tolerance value in Newton-Raphson scheme [-]	IPF	Inverse pole figure
ϕ	Yield function	KAM	Kernel average misorientation
Index Description		MSV	Microstructural state variables
p	Plastic	OES	Optical emission spectroscopy
e	Elastic	PF	Pole figure
d	Deviatoric part	RMV	Representative material volume
v	Volumetric	RMVA	Representative material volume averaging
pc	Plastic stress from cell dislocations	SEM	Scanning electron microscope
		TMM	Thermo-micro-mechanical
		VUMAT	Vectorized user material

capture cumulative deformation effects across manufacturing stages. This model has been validated across cold, warm, and intermediate strain-rate regimes—key ranges for industrial metal forming. Its application in FE simulations of warm-forging an automotive bevel gear made from 20MnCr5 ferritic-pearlitic steel, a material extensively used in

various temperature regimes, further demonstrates its robustness. Studies by Puchi-Cabrera et al. [16,17] and Brnic et al. [18] have corroborated this steel's behavior in these conditions, supporting the model's applicability. Motaman and Prah's approach addresses the complex, temperature- and rate-dependent evolution of dislocation

substructures, specifically dislocation cells and walls [19,20], which drive viscoplastic deformation [21,22]. Their model distinguishes between immobile wall dislocations, which accommodate lattice curvature through geometrically necessary dislocations, and cell dislocations that form metastable boundaries without causing lattice rotation (statistically stored dislocations) [23,24]. These dislocations contribute to short- and long-range back stresses [25], influencing strain hardening and mechanical response. The model also captures the thermally activated dislocation mechanisms that vary across regimes: wall dislocations undergo diffusion-controlled pinning (associated with dynamic strain aging) [26,27], while cell dislocations experience diffusion-controlled climb (linked to creep) [28]. By using dislocation densities as state variables that evolve with temperature and strain rate, the model avoids reliance on empirical plastic strain and enhances predictive capabilities for multiscale modeling in industrial applications [29].

While TMM models effectively capture deformation behavior through dislocation density evolution, their inability to predict material damage limits their effectiveness in simulating processes involving material separation [30–33] and in optimizing multi-step manufacturing sequences to prevent damage from accumulated deformation history [34,35]. Many recent researches has focused on integrating damage prediction into deformation models, employing both empirical [36–42] and phenomenological [43–45] model-based methods. In theoretical modeling, advanced constitutive models have been proposed to simulate thermomechanical behavior, considering interactions between microstructural features and damage. Martínez-Pañeda and Betegón [46] developed a coupled damage model that incorporates strain-gradient plasticity to account for plastic size effects. This integration captures stress elevation and alters plastic zone behavior near crack tips, enhancing fracture predictions in metallic materials. Wu and Zhang [47] introduced a model combining phase-field methods, dislocation-based plasticity, and damage mechanics, specifically tailored for single crystal superalloys. This sophisticated approach provides deeper insights into damage mechanisms in complex materials. In a related development, Zhang et al. [48] presented a dislocation density-based crystal plasticity framework that simulates grain-level plastic deformation and fatigue damage over multiple rolling cycles. Their work elucidates the interactions between microstructural features, such as dislocation densities and grain boundaries, under applied loads, offering a nuanced understanding of material degradation mechanisms. Umantsev's model [49] links microscopic dislocation dynamics to macroscopic damage through a gradient-flow equation, providing a comprehensive view of damage processes. Hu et al. [50] developed a multi-physics, multi-scale framework that integrates thermal-fluid dynamics, phase-field methods, crystal plasticity, and dislocation dynamics to study additively manufactured 316L stainless steel. Their findings demonstrate a strong correlation between regions of high dislocation density and damage nucleation, attributing stress concentrations to dislocation structures formed during the additive manufacturing process. These advancements represent significant progress in modeling the interplay between deformation and damage at the microscopic level, enhancing the predictive capabilities of simulations for complex manufacturing processes. Additional advanced material models for physics-based coupled damage evolution have been proposed in [51,52,53,54,55] etc.

Research underscores the critical influence of dislocation dynamics on material deformation and failure, though a significant limitation persists: most models operate at the microscale, focusing on localized dislocation interactions within grains. Achieving accurate macroscopic simulations requires bridging the gap between microscale dislocation activities and large-scale damage evolution. To advance in this area, modeling efforts should focus on (1) developing a fully integrated constitutive model that incorporates the influence of dislocations on damage initiation and growth, (2) rigorously determining constitutive parameters through experimental investigation and validating model predictions, and (3) applying the model across diverse conditions,

including varied deformation rates, temperatures, and complex loading scenarios. This paper aims to make substantial progress toward these objectives.

Numerous models in the literature integrate micro-level ductile damage mechanisms with hardening behavior for macroscale simulations. Shutov et al. [56] introduced a coupled hardening and damage model utilizing a double multiplicative decomposition of the deformation gradient to address inelastic volume changes from damage, enhancing void nucleation accuracy in complex forming processes. Fil-lafer et al. [57] applied a phenomenological failure criterion accounting for stress concentrations at phase boundaries to pinpoint micro-damage initiation. Wu et al. [58] developed a micromechanical model for C45E + N steel, incorporating microstructural characteristics into a stress-state-dependent damage mechanics model within a crystal plasticity framework. Among many models used, GTN model based on void nucleation, growth and coalescence can accurately predict the tensile ductile fracture, which attracts widespread attentions [59]. For instance, Chen et.al [51] combined the GTN model with a dislocation density-based viscoplasticity model to simulate damage evolution in TWIP steels under surface mechanical treatments. Areias et.al [60] introduced an advanced, robust semi-implicit integration scheme for porous plasticity models, such as the Rousselier and Gurson-Tvergaard-Needleman (GTN) models, under finite strain conditions. Other works done using the GTN model include [61,62,63] etc.

This review also highlights key methods for calibrating GTN damage parameters, focusing on research on S700 steel. H. Xin and M. Veljkovic [64] developed an uncoupled fracture model, calibrated with uniaxial tensile data and validated with notched tests and a triaxially-loaded K-gap joint [65]. Rui Yan et al. applied the GTN model to S355, S500, and S700 steels, using a unit cell approach to investigate fracture under varying triaxialities and calibrating parameters for each grade [62,63]. Other studies, such as Oh et al. [66], used CT specimens to derive initial void fraction parameters from J-R curves, while metallographic analysis has been employed to estimate void and nucleation fractions [67]. The inverse FE approach is frequently used, where damage parameters are iteratively adjusted to align with experimental results from tensile, punch, and other tests [68,69]. Regression methods are also applied; Foad Rahimidehghan et al. [70] used polynomial regression and kriging for GTN parameter prediction. Recently, machine learning, particularly neural networks, has advanced parameter calibration. For example, Paermentier et al. [71] trained a neural network on Charpy-V-Notch simulation data linked to fracture energy, while H. Aguir et al. [72] used blanking process force curves to optimize GTN parameters. These methods highlight a progression toward more data-driven approaches in GTN parameter calibration.

This study introduces a damage-integrated thermo-micro-mechanical (D-TMM) model designed to predict the plastic deformation and ductile damage behavior of S700 steel by accounting for microstructural evolution across various strain rates and temperatures. The model's constitutive parameters were calibrated using force-displacement data from tensile tests under diverse thermal and strain rate conditions. Validation was conducted by comparing the model's predictions with experimental measurements of geometrically necessary dislocation (GND) densities. These densities were obtained from Kernel Average Misorientation (KAM) analyses of Electron Backscatter Diffraction (EBSD) images taken from samples at incremental plastic strains. Results indicate the model's capability to accurately simulate both plastic response and damage progression in S700 steel under tensile loading across a range of temperatures. Unlike traditional multiscale material models, this approach bridges macroscopic and microscopic scales by statistically averaging microstructural features over representative volume elements, enhancing its applicability in macroscopic simulations.

The remaining sections of this paper are organized as follows: [Section 2](#) provides background on microstructural constitutive models and mechanisms of dislocation evolution. [Section 3](#) details key constitutive equations for FE implementation, along with the formulation of a GTN

model integrated with dislocation-based hardening model and modified damage evolution mechanisms. Section 4 outlines the materials and methods used, followed by a detailed calibration process and results for the model parameters, including its physical interpretations. In Section 5, these constitutive parameters are applied in FE simulations of tensile tests under isothermal, non-isothermal, and varying temperature conditions, with accompanying experimental validations, before the paper concludes

2. Background of the TMM model

The dislocation-based multiscale thermo-micro-mechanical model (TMM) is formulated to establish a correlation among stochastic microstructural states (SMS), mesoscale RMVs, and macroscale continuum bodies, as illustrated in Fig. 1. This framework builds upon postulates from Continuum Dislocation Dynamics (CDD) theory, as outlined by Motaman et al., [1] yielding the necessary constitutive relations.

The microstructural constitutive model proposed by Motaman and Prahl [1], grounded in continuum microstructure dynamics (CMD), describes the viscoplastic behavior of metals during deformation. This model has been validated across cold and warm deformation regimes, particularly for case-hardenable steel 20MnCr5. At the macroscale, nonlocal microstructural state variables (MSVs) at each material point are associated with a virtual RMV. These MSVs, representing averaged microstructural features, collectively form the SMS, as introduced by Motaman [1]. The interrelationship between MSVs and macroscopic responses is formalized as:

$$\sigma_y = \bar{\sigma}_y(T, \mathcal{S}, \dot{\epsilon}_p) \quad (1)$$

where σ_y is the nonlocal mean yield stress, or flow stress, which is linked to the mean yield shear stress, $\bar{\tau}_y$, averaged over slip systems and scaled by the Taylor factor [22,23]; $\dot{\epsilon}_p$ represents the mean plastic strain rate; T denotes the temperature; and $\mathcal{S}$ denotes the set of all microstructural state variables (MSVs), collectively referred to as the stochastic microstructural state (SMS). The time evolution of each MSV under thermo-mechanical loading is given by:

$$\dot{\mathcal{S}}_k = \dot{\mathcal{S}}_k(T, \mathcal{S}, \dot{\epsilon}_p) \quad (2)$$

where $\dot{\mathcal{S}}_k$ denotes the time rate of change of the k^{th} MSV. The set $\mathcal{S}$ denotes the microstructural state of a material point within a macroscale continuum body, as shown in Fig. 1, and evolves with deformation [29].

Dislocations within crystal grains distribute heterogeneously and can be classified into two primary types based on their spatial arrangement: cell dislocations and wall dislocations. Fig. 2 illustrates the cell-wall substructure within crystal grains. In which, cell dislocations within cell or subgrain blocks are generally mobile, lacking structured

arrangements, and are statistically distributed within the cell block (CB) structure, hence referred to as statistically stored dislocations (SSDs) [73]. Conversely, immobilized cell dislocations aggregate into semi-temporary clusters known as incidental dislocation boundaries (IDBs) [74]. Geometrically necessary dislocations (GNDs), arising from lattice distortions induced by plastic strains [75,76] are called wall dislocations, which generate measurable misorientation angles and are detectable via electron backscatter diffraction (EBSD) and X-ray analysis [77].

Within the framework of the CDD-based TMM model, dislocation densities serve as MSVs, categorized by mobility (mobile vs. immobile) and spatial organization (cell vs. wall dislocations) [20]. Mobile dislocations primarily facilitate plastic deformation, while immobile dislocations contribute to plastic hardening [78,79]. The movement of mobile dislocations may be impeded, transforming them into immobile dislocations.

Three primary, independent types of dislocation density are thus identified: cell mobile dislocation density ρ_{cm} , cell immobile dislocation density ρ_{ci} , and wall immobile dislocation density ρ_{wi} , which are grouped as microstructural state as:

$$\mathcal{S} \equiv \{\rho_{cm}, \rho_{ci}, \rho_{wi}\}; \quad (3)$$

$$\rho_{SS} = \rho_{cm} + \rho_{ci}$$

$$\rho_{GND} = \rho_{wi} \quad (4)$$

The densities of mobile and immobile dislocations at each macroscale material point are defined as follows:

$$\rho_{cm} = \frac{1}{V} \sum_j l_{cm}^{(j)}; \rho_{ci} = \frac{1}{V} \sum_j l_{ci}^{(j)}; x = c, w \quad (5)$$

where V is the considered nonlocal volume, corresponding to the volume of mesoscale RMV; $l_{cm}^{(j)}$ and $l_{ci}^{(j)}$ denote the lengths of j^{th} mobile dislocation and immobile dislocation segments (x), respectively; and ρ_{cm} and ρ_{ci} refer to the nonlocal mobile and immobile dislocation densities. Here, x can be either c or w , indicating cell and wall dislocations, respectively. Under deformation, these dislocations evolve through dynamic and static processes, summarized in Table 1.

3. Constitutive equations

3.1. Constitutive theory of isotropic hypoelasto-viscoplastic finite deformation

The constitutive theory for isotropic hypoelasto-viscoplastic (HEVP) finite deformation models material behavior under applied forces, incorporating both elastic and plastic responses within a finite deformation framework. This theory spans core concepts, including kinematics, elastoplastic decomposition, polar decomposition, corotational

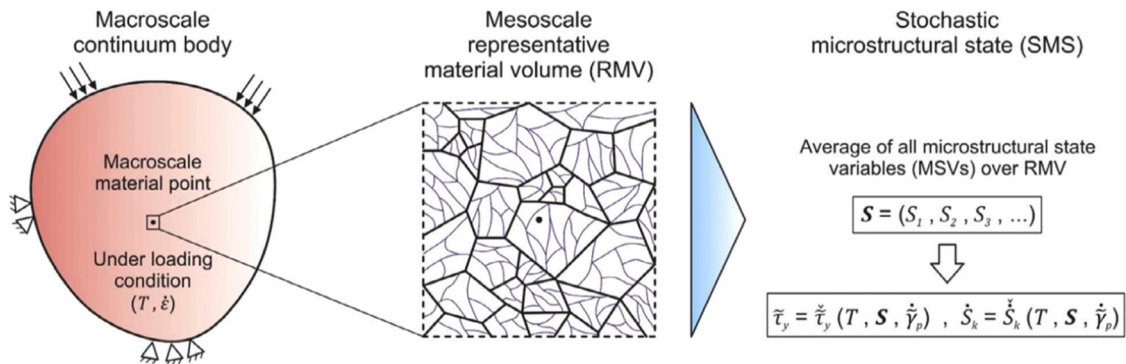


Fig. 1. Schematic relationship between the macroscopic continuum body under thermo-mechanical loading, mesoscale representative material volume and stochastic microstructural state [1].

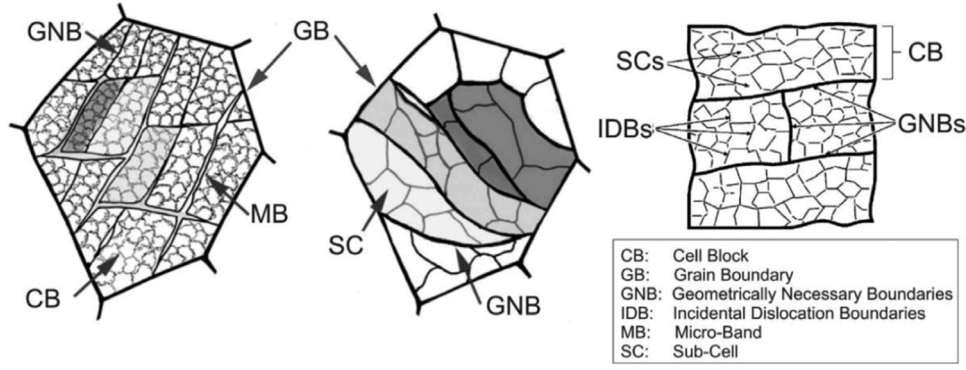


Fig. 2. Illustration of grain subdivision to cell-wall dislocation microstructure [1].

formulation, constitutive relations, and volumetric-deviatoric decomposition. Together, these subsections provide a unified approach to understanding and modeling material deformation under complex loading.

3.1.1. Kinematics of Deformation

Kinematics lays the groundwork for describing material deformation by tracking particle movement. A material body initially occupies configuration Ω_0 , with each particle P positioned at coordinate X . Upon deformation, P moves to a new position P' , with updated coordinate x and displacement $\underline{U} = \underline{u}$. For a neighboring particle Q , initially separated by dX , this distance becomes dx in the deformed state. The deformation gradient is computed by:

$$d\underline{x} = \underline{F} \cdot d\underline{X}; \quad \underline{F} = \frac{\partial \underline{x}(\underline{X})}{\partial \underline{X}}; \quad (6)$$

where the deformation gradient tensor $\underline{F}$ connects the displacements between the initial and deformed configurations. The velocity gradient tensor $\underline{L}$ represents the rate of change of the displacement vector:

$$\underline{v} = \frac{\partial \underline{u}}{\partial t} = \frac{\partial \underline{x}}{\partial t}. \quad (7)$$

The velocity gradient tensor $\underline{L}$ can be decomposed into the symmetric rate of deformation tensor $\underline{D}$ and the skew-symmetric spin tensor $\underline{W}$, which quantify the deformation process.

$$\underline{L} = \underline{D} + \underline{W}; \quad \underline{D} = \text{sym}(\underline{L}) = \frac{1}{2}(\underline{L} + \underline{L}^T); \quad \underline{W} = \text{skw}(\underline{L}) = \frac{1}{2}(\underline{L} - \underline{L}^T) \quad (8)$$

This decomposition helps in understanding and analyzing material behaviors that are due to deformation (e.g., inelastic deformation, plastic flow) versus those due to rotation (e.g., spin, rigid body rotation).

3.1.2. Polar Decomposition of Deformation Gradient

The polar decomposition theorem allows any non-singular second-order tensor, such as the deformation gradient $\underline{F}$, to be expressed as a product of an orthogonal rotation tensor $\underline{R}$ and a symmetric stretch tensor $\underline{U}$:

$$\underline{F} = \underline{R}\underline{U} = \underline{V}\underline{R}; \quad (9)$$

where $\underline{R}$ represents the rigid-body rotation, and $\underline{U}$ and $\underline{V}$ describe right and left stretches, respectively, with $\underline{U}^2 = \underline{C} = \underline{F}^T \underline{F}$ and $\underline{V}^2 = \underline{B} = \underline{F} \underline{F}^T$, where $\underline{B}$ and $\underline{C}$ are left and right Cauchy-Green deformation tensors, respectively. This decomposition aids in separating deformation into rotation and stretch components, supporting analyses of changes in orientation and shape.

3.1.3. Elastoplastic decomposition of deformation gradient

In elastoplastic theory, the total deformation gradient $\underline{F}$ is decomposed into elastic $\underline{F}_e$ and plastic $\underline{F}_p$ components [97]:

$$\underline{F} = \underline{F}_e \underline{F}_p. \quad (10)$$

Given the small elastic strain rates in hypoelasto-viscoplastic materials [29,98], the total $\underline{L}$ is approximated as:

$$\underline{L} \approx \underline{L}_e + \underline{L}_p; \quad \underline{D} = \underline{D}_e + \underline{D}_p; \quad \underline{W} = \underline{W}_e + \underline{W}_p; \quad (11)$$

where $\underline{L}_e$ and $\underline{L}_p$ represent elastic and plastic velocity gradients, respectively. These gradients further decompose into symmetric tensors $\underline{D}_e$, $\underline{D}_p$ and skew symmetric tensors $\underline{W}_e$, $\underline{W}_p$. The strain rate measure is the power conjugate of Cauchy stress tensor [29], denoted as:

$$\dot{\epsilon} = \dot{\epsilon}_e + \dot{\epsilon}_p; \quad \dot{\epsilon} \equiv \dot{D}; \quad \dot{\epsilon}_e \equiv \dot{D}_e; \quad \dot{\epsilon}_p \equiv \dot{D}_p \quad (12)$$

where $\dot{\epsilon}$, $\dot{\epsilon}_e$, $\dot{\epsilon}_p$ are respectively total, elastic and plastic strain rate tensors. This decomposition is essential for modeling hypoelastic-viscoplastic behavior under load.

3.1.4. Corotational formulation

The corotational formulation addresses rotational effects, critical for analyzing realistic material behaviors under rotation. The material point's rotation is represented by an orthogonal rotation tensor $\underline{R}$, evolving as:

$$\dot{\underline{R}} = \underline{\Omega} \underline{R}; \quad \underline{R}_0 = \underline{I}; \quad \underline{R}^{-1} = \underline{R}^T; \quad (13)$$

where $\underline{\Omega}$ is a skew-symmetric tensor associated with $\underline{R}$, defined by $\underline{\Omega} = \dot{\underline{R}} \underline{R}^T$. In this corotational configuration, the symmetric Cauchy stress tensor $\underline{\sigma}$ is transformed as:

$$\hat{\sigma} = \underline{R}^T \cdot \underline{\sigma} \cdot \underline{R} \quad (14)$$

where $\hat{\sigma}$ represents the rotated, corotational form of the stress tensor. Similarly, the corotated deformation rate tensor is given by:

$$\hat{D} = \underline{R}^T \cdot (\underline{D}_e + \underline{D}_p) \cdot \underline{R} = \hat{D}_e + \hat{D}_p. \quad (15)$$

The time derivative of the rotated Cauchy stress tensor follows:

$$\dot{\hat{\sigma}} = \underline{R}^T \cdot \dot{\underline{\sigma}} \cdot \underline{R}. \quad (16)$$

3.1.5. Constitutive relations

In the HEVP framework, constitutive relations link stress and strain based on Hooke's law and material objectivity (the invariance of material response under changes in observer frames) as:

$$\dot{\hat{\sigma}} = \mathbb{C}_{ijkl}^e : \dot{\epsilon}_e = \mathbb{C}_{ijkl}^e : (\dot{\epsilon} - \dot{\epsilon}_p) \quad (17)$$

where $\hat{\sigma}$ is the material objective Cauchy stress tensor; $\mathbb{C}_{ijkl}^e$ is the elastic

Table 1

Static and dynamic dislocation mechanisms considered in the TMM model.

Process type	Description	Mechanism	References
Annihilation of dislocations	Mobile dislocations with opposite burger vector annihilate the other types on neighboring slip planes.	Thermally activated dislocation climb and cross slip mechanisms	[80–83]
Accumulation of immobile dislocations	Mobile dislocations are immobilized by immobile dislocations, thereby increasing immobile dislocations.	Athermal process	[1]
Generation of mobile dislocations	Motion of mobile dislocations, thereby the length of the mobile dislocation increases.	Frank-Read mechanism Cross slip mechanism Mobile junction mechanism	[84–87]
Nucleation of wall dislocations	Accumulated cell immobile dislocation will become wall immobile if the immobilization is strong, exceeds critical size & density.	Local stress concentration at IDBs results in GNBs or wall dislocations in metals with low SFE; Thermally active process.	[88–90]
Remobilization of immobile dislocations	Immobile dislocations can be mobilized and thus resulting in plastic straining.	Due to climbing, cross-slips, bow-out, junction dissociation etc. Thermally activated processes such as climb and cross-slip. Lomer-Cottrell lock junctions Hirth lock junctions Coplanar lock junctions	[79]
Trapping of mobile dislocations	Interaction of mobile dislocations with each other could immobilize the dislocations. If the immobilization takes place due to the pinning by interstitial atoms, it is called pinning and if it's caused by the locking of mobile dislocations, results in dynamic strain Ageing (DSA).		[91–95]
Static pinning of cell dislocations	Pinning of cell dislocations due to the diffusion of interstitial atoms to the statistically distributed dislocation cores and junctions.		[96]
Static remobilization	Due to thermal mechanisms such as dislocation climb and junction dissociation.		[1]

stiffness tensor, defined as a function of the elastic, shear, and bulk moduli. In isotropic linear elastic materials, the fourth-order isotropic tensor is:

$$C_{ijkl} = 2G\delta_{ij}\delta_{kl} + \left(K - \frac{2}{3}G\right)\delta_{ij}\delta_{kl}, \text{ when } x = y, \delta_{xy} = 1 \text{ else } \delta_{xy} = 0 \quad (18)$$

where G and K are Shear modulus and Bulk modulus. This section provides a basis for determining material stress responses across elastic and plastic regimes.

3.1.6. Volumetric-deviatoric decomposition

The strain rate tensor is decomposed into volumetric and deviatoric parts,

$$\dot{\epsilon} = \dot{\epsilon}^v + \dot{\epsilon}^d; \dot{\epsilon}^v = \dot{\epsilon} : \mathbf{I}; \dot{\epsilon}^d = \dot{\epsilon} - \frac{1}{3}\dot{\epsilon}^v \mathbf{I} \quad (19)$$

where ϵ^v and ϵ^d are volumetric and deviatoric strains, respectively, allowing separation of volume-preserving and shape-altering strain behaviors. These terms are further divided into their elastic and plastic components, supporting analysis of strain under conditions where compressibility affects material softening. By knowing the equivalence of hydrostatic parts of objective and spatial time derivatives of stress (due to proportionality to the first invariant of stress rate tensors), the objective stress rate (from Eq. (17)) decomposes as:

$$\dot{\hat{\sigma}} = \dot{\hat{\sigma}}_h + \dot{\hat{\sigma}}_d, \quad (20)$$

where $\dot{\hat{\sigma}}_h = \frac{1}{3}\mathbf{I} : \dot{\sigma}$ and $\dot{\hat{\sigma}}_d$ are the hydrostatic and deviatoric stress rate contributions, respectively. Applying this provides a complete representation of stress in a fixed spatial frame:

$$\dot{\hat{\sigma}}_h = K\dot{\epsilon}^v \mathbf{I}; \dot{\hat{\sigma}}_d = 2G\dot{\epsilon}^d; \quad (21)$$

$$\dot{\hat{\sigma}} = \mathbb{C}_{ijkl}^e : \dot{\epsilon}_e = 2G\dot{\epsilon}_e + \left(K - \frac{2}{3}G\right)\dot{\epsilon}^v \mathbf{I}; \quad (22)$$

$$\sigma = \sigma_h + \sigma_d; \sigma_h = \frac{1}{3}\mathbf{I} : \sigma; \sigma_d = \sigma - \sigma_h. \quad (23)$$

Along with isotropic plasticity criteria and corotational formulations, form the framework for HEVP, enabling accurate prediction of material responses under complex loading.

3.2. Microstructural constitutive model

The yield stress σ_y in isotropic viscoplasticity consists of two primary components: the rate-independent plastic stress σ_p and a rate-dependent viscous stress σ_v , expressed as:

$$\sigma_y = \sigma_p + \sigma_v. \quad (24)$$

Plastic hardening arises from the density of immobile dislocations, with σ_p decomposed into contributions from cell and wall immobile dislocations [99,100]:

$$\sigma_p = \sigma_{pc} + \sigma_{pw}, \quad (25)$$

where σ_{pc} and σ_{pw} represent stresses from cell and wall dislocation densities, respectively. Based on the Taylor equation, these stress contributions relate to dislocation densities as [101,102]:

$$\sigma_{px} = MbG\tilde{\alpha}_x\sqrt{\rho_{xi}}; x = c, w \quad (26)$$

where σ_{px} is derived from immobile dislocations of type x ; ρ_{xi} is the corresponding immobile dislocation density; $\tilde{\alpha}_x$ is the nonlocal interaction strength; b is the Burgers vector; G is the shear modulus, and M is the Taylor factor. The viscous stress σ_v reflects resistance to dislocation motion in an obstacle-free lattice, influenced by strain rate and temperature:

$$\sigma_v = \sigma_{v0}\hat{\epsilon}_p^{m_v}; \sigma_{v0} = \sigma_{v00}[1 + r_v(\hat{T} - 1)^{s_v}]; \quad (27)$$

$$\hat{T} \equiv \frac{T}{T_0}; \hat{\epsilon}_p \equiv \frac{\dot{\epsilon}_p}{\dot{\epsilon}_0}; r_v < 0; 0 < s_v \leq 1$$

where m_v is the strain rate sensitivity, and parameters $r_v < 0$ and $0 < s_v \leq 1$ define temperature sensitivity. The combination of shear modulus and mean interaction strengths $G\tilde{\alpha}_x$ from Eq. (26) and viscous strain rate exponent m_v (in Eq. (27)) depends on temperature and strain rate:

$$\dot{G}\tilde{\alpha}_x = G_0\tilde{\alpha}_{x0}\left[1 + r_{ax}^G(\hat{T} - 1)^{s_{ax}^G}\right]; r_{ax}^G \langle 0; s_{ax}^G \rangle 0; x = c, w; \quad (28)$$

$$m_v = m_{v0}\left[1 + r_v^m(\hat{T} - 1)^{s_v^m}\right]\dot{\epsilon}_p^m; r_v^m, s_v^m \geq 0; \quad (29)$$

where r_{ax}^G and s_{ax}^G are temperature sensitivity coefficient and exponent associated with $\dot{G}\tilde{\alpha}_x$; m_{v0} is the reference strain rate sensitivity (obtained at reference temperature and strain rate); r_v^m and s_v^m are temperature sensitivity coefficient and exponent associated with strain rate sensitivity of viscous stress; and m_v^m is the strain rate sensitivity parameter associated with strain rate sensitivity of viscous stress.

As a material undergoes plastic deformation, it experiences strain hardening due to the dynamic evolution of dislocation density. This evolution, or rate of change in dislocation density with respect to plastic strain, arises from a balance of dislocation creation and annihilation via several physical mechanisms (Table 1) within the material [103,104]. The evolution of dislocation densities—including cell immobile, cell mobile, and wall immobile dislocations—and the associated mechanisms are outlined in Section 3.2.1. For calculation convenience, dimensionless dislocation densities are used:

$$\hat{\rho}_{xy} \equiv \frac{\rho_{xy}}{\rho_0}; \begin{cases} x = c, w \\ y = m, i \end{cases} \quad (30)$$

where c represents cell; w represents wall; m represents mobile, and i represents immobile dislocations.

3.2.1. Evolution of dislocation densities

The net increase in the wall immobile dislocation density is due to nucleation of new wall immobile dislocations due to the pile-up of cell immobile dislocations over a critical size forming dense wall like structure and due to the accumulation of mobile dislocations, whereas the decrease in the wall immobile dislocations will be due to mutual annihilation of cell mobile and wall immobile dislocations with respect to the plastic shear increment. The net change in the wall immobile dislocations during plastic deformation is:

$$\dot{\hat{\rho}}_{wi} = \dot{\hat{\rho}}_{wi}^{nc} + \dot{\hat{\rho}}_{wi}^{ac} + (-\dot{\hat{\rho}}_{wi}^{an} - \dot{\hat{\rho}}_{wi}^{rm}). \quad (31)$$

Similarly, new cell immobile dislocations are formed due to trapping of cell mobile dislocations in Lomer-Cottrell lock junctions [91,94] and due to accumulation of cell mobile dislocations. The net density of cell immobile dislocations decreases due to their pile-up into wall structures, mutual annihilation with mobile dislocations, and remobilization back to a mobile state. The net change is given as:

$$\dot{\hat{\rho}}_{ci} = \dot{\hat{\rho}}_{ci}^{tr} + \dot{\hat{\rho}}_{ci}^{ac} + (-\dot{\hat{\rho}}_{ci}^{an} - \dot{\hat{\rho}}_{ci}^{rm} - \dot{\hat{\rho}}_{ci}^{nc}). \quad (32)$$

Mobile dislocations are generated through mechanisms such as the Frank-Read source [84], multiple cross-slip [85], and mobile junction formation [86]. Remobilization of cell and wall immobile dislocations further increases mobile dislocation density. However, the overall mobile dislocation density decreases due to mutual annihilation with cell and wall immobile dislocations, self-annihilation, accumulation into immobile forms, and trapping from interactions across different slip planes [1]. The net change in mobile dislocation density with plastic strain increment is given as:

$$\dot{\hat{\rho}}_{cm} = \dot{\hat{\rho}}_{cm}^{gn} + \dot{\hat{\rho}}_{cm}^{rm} + \dot{\hat{\rho}}_{cm}^{tr} + (-2\dot{\hat{\rho}}_{cm}^{an} - \dot{\hat{\rho}}_{ci}^{an} - \dot{\hat{\rho}}_{wi}^{an} - \dot{\hat{\rho}}_{ci}^{ac} - \dot{\hat{\rho}}_{wi}^{ac} - \dot{\hat{\rho}}_{ci}^{tr}). \quad (33)$$

The evolution of dislocation densities owing to different physical mechanism ($\dot{\hat{\rho}}_{xy}^z$) can be expressed as:

$$\dot{\hat{\rho}}_{cm}^{gn} = M c_{cm}^{gn} \frac{\hat{\rho}_{cm}}{\sqrt{\hat{\rho}_{ci} + \hat{\rho}_{wi}}} \dot{\epsilon}_p;$$

$$\dot{\hat{\rho}}_{xy}^{an} = M c_{xy}^{an} \hat{\rho}_{cm} \hat{\rho}_{xy} \dot{\epsilon}_p; xy = cm, ci, wi;$$

$$\dot{\hat{\rho}}_{xi}^{ac} = M c_{xi}^{ac} \sqrt{\hat{\rho}_{xi}} \hat{\rho}_{cm} \dot{\epsilon}_p; x = c, w;$$

$$\dot{\hat{\rho}}_{cm}^{tr} = M c_{cm}^{tr} \hat{\rho}_{cm}^{3/2} \dot{\epsilon}_p;$$

$$\dot{\hat{\rho}}_{wi}^{nc} = M c_{wi}^{nc} \hat{\rho}_{ci}^{3/2} \hat{\rho}_{cm} \dot{\epsilon}_p;$$

$$\dot{\hat{\rho}}_{xi}^{rm} = M c_{xi}^{rm} \hat{\rho}_{xi} \dot{\epsilon}_p; x = c, w; \quad (34)$$

where the superscripts gn , an , ac , tr , nc and rm denote the dynamic dislocation evolution processes: generation, annihilation, accumulation, trapping, nucleation, and remobilization, respectively. The parameter c_{xy}^z represents the constitutive parameter associated with the probability amplitude or frequency of occurrence of dislocation process z (gn , an , ac , tr , nc , rm) for dislocations of type $xy(cm, ci, wi)$.

Most constitutive parameters are temperature- and strain rate-dependent, as thermally activated and diffusion-controlled mechanisms, such as Peierls and cross-slip, influence dislocation behaviour. To account for these effects, the constitutive parameter for each mechanism is expressed as:

$$c_{xy}^z = c_{xy0}^z \left[1 + r_{xy}^z(\hat{T} - 1)^{s_{xy}^z}\right] \dot{\epsilon}_p^{m_{xy}^z}; xy = cm, ci, wi;$$

$$m_{xy}^z = m_{xy0}^z \left[1 + r_{zxy}^m(\hat{T} - 1)^{s_{zxy}^m}\right]; xy = cm, ci, wi; \quad (35)$$

where c_{xy0}^z is the material constant obtained at the reference temperature and strain rate, representing the probability amplitude of the dislocation process z involving dislocations of type xy . The parameters r_{xy}^z and s_{xy}^z denote the temperature sensitivity coefficient and exponent, respectively, associated with this probability amplitude; Similarly, m_{xy0}^z is the reference strain rate sensitivity for the process, while r_{zxy}^m and s_{zxy}^m are temperature sensitivity coefficient and exponent associated with the strain rate sensitivity of the dislocation process z involving dislocations of type xy [29].

3.3. Yield function – Gurson Tvergaard and Needleman (GTN) model

The von Mises yield criterion is used in the existing works which considered the microstructural constitutive model for the hardening behavior [1]. This yield criterion is independent of the hydrostatic stress [105] and can be expressed as:

$$\phi \equiv \sigma_{eq} - \sigma_y$$

$$\sigma_y \equiv \sigma_y(T, S, \dot{\epsilon}_p) \text{ and } \sigma_{eq} \equiv \sigma_{eq}(\sigma) = \sqrt{3J_2(\sigma)} = \sqrt{\frac{3}{2} \|s_{ij}\|}; \quad (36)$$

where σ_{eq} is the equivalent (von Mises) stress; σ_y is the yield stress calculated using microstructural constitutive model; T is the temperature; $\dot{\epsilon}_p$ is the equivalent (von Mises) plastic strain rate and $J_2(\sigma)$ is the second invariant of deviatoric part s_{ij} of the Cauchy stress tensor.

Hydrostatic stress is a critical factor in damage accumulation processes such as void nucleation, growth, and coalescence, which are key mechanisms in ductile fracture. Elevated hydrostatic stresses facilitate the formation and expansion of micro voids or microcracks within the material, ultimately contributing to progressive degradation and potential failure. Since the von Mises criterion excludes hydrostatic stress effects, it does not accurately capture the onset and evolution of damage, limiting its suitability in applications involving cumulative damage.

Ductile fracture initiates with void formation and growth within the metal matrix, which in turn influences hydrostatic stress. Gurson developed a yield function to account for void effects on yielding behavior [106]. This function models the response of a representative volume element comprising an incompressible, homogeneous, rigid plastic von Mises matrix with a spherical void. Tvergaard and

Needleman later refined Gurson's model to improve its representation of void effects in yielding behavior [107] as:

$$\phi = \left(\frac{\sigma_{eq}}{\sigma_y}\right)^2 + 2q_1 f^* \cosh\left(\frac{-3q_2 \sigma_h}{2\sigma_y}\right) - (1 + q_3 f^{*2}) = 0 \quad (37)$$

where ϕ is the gurson yield function; σ_{eq} is the equivalent (von Mises) stress; σ_y is the yield stress calculated using microstructural constitutive model; f^* is the modified/ effective void fraction accounting for the accelerating effects of the void coalescence; σ_h is the hydrostatic stress. The parameters q_1 , q_2 and q_3 are additional parameters proposed by Tvergaard [108,109] to reconcile the results of the Gurson equations with the numerical studies. The modified void fraction is given as:

$$f^* = \begin{cases} f & \text{if } f \leq f_c \\ f_c + \frac{f_u - f_c}{f_f - f_c} (f - f_c) & \text{if } f > f_c \end{cases}, \quad (38)$$

where f_c is the critical void volume fraction at which void coalescence begins; f_f is the failure fraction; f_u^* is the material parameter, calculated by $f_u^* = 1/q_1$. The evolution of the total volume fraction of voids due to plastic strain increment is given by:

$$\dot{f} = \dot{f}_{nucl} + \dot{f}_{growth}, \quad (39)$$

where $\dot{f}$ is the rate of change of total void volume fraction with respect to time; $\dot{f}_{nucl}$ is the rate of increase in void volume fraction due to nucleation with respect to time and $\dot{f}_{growth}$ is the rate of increase in void volume fraction due to growth with respect to time. The void fraction increase due to nucleation is dependent on the equivalent plastic strain increment:

$$\dot{f}_{nucl} = A_N \bar{\epsilon}_p;$$

$$A_N \equiv A_N(\bar{\epsilon}_p) \equiv \frac{f_N}{S_N \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{\bar{\epsilon}_p - \epsilon_N}{S_N}\right)^2\right] \quad (40)$$

where f_N and S_N are the nucleated volume fraction and gaussian standard deviation; ϵ_N is the mean equivalent plastic strain at which the nucleation starts. As the void fraction increases during plastic deformation, plastic dilation occurs, resulting in permanent material expansion. This effect arises from the influence of hydrostatic stress, and the relationship between void growth and hydrostatic stress is expressed as:

$$\dot{f}_{growth} = (1 - f) \dot{\epsilon}_p : \mathbf{I}. \quad (41)$$

Thus, the overall evolution of the total void volume fraction due to plastic strain increment is:

$$\dot{f} = \dot{f}_{nucl} + \dot{f}_{growth}. \quad (42)$$

3.3.1. Flow rule

The flow rule defines the essential relationship between the plastic strain rate and the yield surface gradient, enabling accurate descriptions of material behavior under plastic deformation. By establishing this connection, the flow rule provides a basis for determining the direction and magnitude of plastic strain increment, acting as a key factor in modeling material response to different loading conditions. This relationship is expressed as follows:

$$\dot{\epsilon}_p = \dot{\lambda} \frac{\partial \psi}{\partial \sigma} = \dot{\lambda} \frac{\partial \phi}{\partial \sigma} = \dot{\lambda} \underline{n}; \underline{n} \equiv \frac{\partial \phi}{\partial \sigma}; \quad (43)$$

where $\dot{\lambda}$ is the non-negative consistency parameter or viscoplastic multiplier; $\underline{n}$ is known as flow direction tensor, which represents yield surface normal tensor [29]. The macroscopic plastic strain $\dot{\epsilon}_p$ (can also be expressed in incremental form $\Delta \epsilon_p$) can be determined through this relationship:

$$\Delta \epsilon_p = \Delta \lambda \left(\frac{\partial \phi}{\partial \sigma} \underline{n} + \frac{1}{3} \frac{\partial \phi}{\partial \sigma_h} \mathbf{I} \right); \Delta \lambda \left(\frac{\partial \phi}{\partial \sigma_h} \right) = \Delta \epsilon_p^v; \Delta \lambda \left(\frac{\partial \phi}{\partial \sigma} \right) = \Delta \epsilon_p^d; \quad (44)$$

where $\underline{n} = \frac{3}{2} \frac{\epsilon_p^d}{\bar{\epsilon}_p}$; $\Delta \epsilon_p^v$ and $\Delta \epsilon_p^d$ are the mean plastic strain increment and equivalent plastic strain increment, the interrelationship between them can be obtained as (from Eq. (44)):

$$\Delta \epsilon_p^v \frac{\partial \phi}{\partial \sigma} = \Delta \epsilon_p^d \frac{\partial \phi}{\partial \sigma_h}. \quad (45)$$

The plastic strain increment can be written as:

$$\Delta \epsilon_p = \frac{1}{3} \Delta \epsilon_p^v \mathbf{I} + \Delta \epsilon_p^d \underline{n}. \quad (46)$$

3.3.2. Equivalent Plastic Work Principle

The macroscopic plastic strain rate $\dot{\epsilon}_p$ is linked to the microscopic equivalent plastic strain rate $\dot{\bar{\epsilon}}_p$ of the matrix material by using the equivalent plastic work principles such as:

$$(1 - f) \sigma_y \dot{\bar{\epsilon}}_p = \underline{\sigma} : \dot{\epsilon}_p; \quad (47)$$

where σ_y is the yield stress of the matrix material and $\underline{\sigma}$ is the Cauchy stress tensor. The damage-integrated microstructural model is complete with the inclusion of the Kuhn-Tucker (loading-unloading) complementary conditions:

$$\dot{\lambda} \geq 0, \quad \phi \leq 0, \quad \dot{\lambda} \phi = 0. \quad (48)$$

The consistency condition for loading-unloading is $\dot{\lambda} \phi = 0$.

3.4. Numerical integration and algorithmic procedure

The finite element implementation of the Gurson yield function has been widely explored by various researchers [110–112], with most studies employing empirical hardening functions to represent the material's yield behavior [70,113–116]. This study progresses these efforts by incorporating microstructural state variables (MSVs) to model material hardening and softening dynamics through the evolution of dislocation density and void fraction.

To account for damage evolution, the Gurson yield function is integrated into ABAQUS/Explicit via a custom VUMAT subroutine. The explicit time integration in ABAQUS/Explicit is particularly suited for non-linear dynamic problems [117], where the total simulation time is divided into small increments Δt ($t^{(n)} \rightarrow t^{(n+1)}$) to ensure accurate time-stepping and stability in dynamic analyses. The yield function at the end of each step increment is given as:

$$\phi^{n+1}(\sigma_y^{n+1}, \bar{\sigma}^{n+1}, \sigma_h^{n+1}, \mathbf{S}) = 0. \quad (49)$$

3.4.1. Elastic predictor step/ trial step

During the elastic predictor (trial) step, it is assumed that only elastic deformation occurs ($\dot{\epsilon}_p^{(n+1)} = 0$). Thus, the trial stress is:

From Eq. (17),

$$\underline{\sigma}_{trial}^{(n+1)} = \underline{\sigma}^{(n)} + \Delta \underline{\sigma}_{trial}^{(n+1)} \quad (50)$$

$$\underline{\sigma}_{trial}^{(n+1)} = \mathbb{C}_{ijkl}^e : \dot{\underline{\epsilon}}_{trial}^{(n+1)} = \mathbb{C}_{ijkl}^e : \dot{\underline{\epsilon}}^{(n+1)}; \quad (51)$$

where $\dot{\underline{\epsilon}}^{(n+1)}$ is the total strain increment. For isotropic materials, this can be further expressed as (based on Eq. (18)):

$$\underline{\sigma}_{trial}^{(n+1)} = 2G \dot{\underline{\epsilon}}^{(n+1)} + \left(K - \frac{2}{3}G\right) \dot{\epsilon}^{(n+1)} \mathbf{I}; \quad (52)$$

$$\sigma_{trial}^h = \frac{1}{3} \underline{\sigma}_{trial}^{(n+1)} : \mathbf{I}; \quad (53)$$

$$\underline{\sigma}_{trial}^d = \underline{\sigma}_{trial}^{(n+1)} - \sigma_{trial}^h \mathbf{I}. \quad (54)$$

where σ_{trial}^h and $\underline{\sigma}_{trial}^d$ are trial hydrostatic stress and trial deviatoric stress. Considering Eq. (43), the trial flow stress reads:

$$\underline{n} = \frac{3}{2} \frac{\underline{\sigma}^d}{\bar{\sigma}} = \frac{3}{2} \frac{\underline{\sigma}_{trial}^d}{\bar{\sigma}_{trial}} \Rightarrow \underline{\sigma}_{trial}^d = \frac{2}{3} \bar{\sigma}_{trial} \underline{n}. \quad (55)$$

The equivalent stress can be calculated from the deviatoric stress as:

$$\bar{\sigma} = \sqrt{\frac{3}{2} \|\underline{\sigma}^d\|} \Rightarrow \underline{\sigma}^d = \frac{2}{3} \bar{\sigma} \Rightarrow \underline{\sigma}_{trial}^d = \frac{2}{3} \bar{\sigma}_{trial}. \quad (56)$$

3.4.2. Plastic corrector with return mapping

If the trial stress state surpasses the yield condition, a plastic corrector step is applied, modifying the trial stress to satisfy the yield function. Corrected stress components are calculated by:

Substituting Eq. (17) in Eq. (50):

$$\Delta \underline{\sigma}^{(n+1)} = \Delta \underline{\sigma}_{trial}^{(n+1)} - \mathbf{C}_{ijkl}^e : \underline{\varepsilon}_p^{(n+1)}. \quad (57)$$

Using the expansions from Eq. (21) in Eq. (50):

$$\Delta \underline{\sigma}^{(n+1)} = \Delta \underline{\sigma}_{trial}^{(n+1)} - K \Delta \varepsilon_p^{(n+1)} - 3G \Delta \varepsilon_p^d^{(n+1)}. \quad (58)$$

Thus, by equating the expressions from both sides, the equations for plastic correction are given as:

$$\sigma^{h(n+1)} = \sigma_{trial}^h - K \Delta \varepsilon_p^{(n+1)} \quad (59)$$

$$\bar{\sigma}^{(n+1)} = \bar{\sigma}_{trial} - 3G \Delta \varepsilon_p^d^{(n+1)} \quad (60)$$

where $\Delta \varepsilon_p^{(n+1)}$ and $\Delta \varepsilon_p^d^{(n+1)}$ must be calculated for each increment for plastic correction, from the relationships obtained in Eq. (44):

$$\Delta \varepsilon_p^{(n+1)} = \Delta \lambda^{(n+1)} \left(\frac{\partial \phi}{\partial \sigma_h} \right)_{n+1} = 3q_1 q_2 f^{(n+1)} \sigma_y^{(n+1)} \Delta \lambda^{(n+1)} \sinh \left(\frac{3q_2 \sigma_h^{(n+1)}}{2\sigma_y^{(n+1)}} \right); \quad (61)$$

$$\Delta \varepsilon_p^d^{(n+1)} = \Delta \lambda^{(n+1)} \left(\frac{\partial \phi}{\partial \bar{\sigma}} \right)_{n+1} = 2\bar{\sigma}^{(n+1)} \Delta \lambda^{(n+1)} \quad (62)$$

$$\bar{\sigma}^{(n+1)} = \frac{\bar{\sigma}_{trial}}{(1 + 6G \Delta \lambda^{(n+1)})}. \quad (63)$$

At the end of each correction step, the yield function $\phi_{trial}^{(n+1)}$ is calculated to check if the Kuhn-Tucker complementary conditions are satisfied according to Eq. (48):

$$\phi_{trial}^{(n+1)} \begin{cases} \leq 0 : \text{Elastic step} \\ > 0 : \text{Plastic step} \end{cases} \quad (64)$$

If the plastic step exists (according to Eq. (64)), then the stress-based return mapping approach is used as plastic corrector, the yield function along with a set of other functions (associated with the unknowns such as MSVs and plastic multiplier) will be solved simultaneously for the plastic strain increment, stress tensor and MSVs.

3.4.3. Integration procedure

Forward/explicit Euler method for numerical integration of normalized dislocation density and void fraction is given as:

$$\hat{\rho}_{xy}^{(n+1)} = \hat{\rho}_{xy}^{(n)} + \Delta \hat{\rho}_{xy}^{(n)}; \Delta \hat{\rho}_{xy}^{(n)} = \Delta \varepsilon_p^{(n+1)} \partial_{\varepsilon_p} \hat{\rho}_{xy}^{(n+1)} = \Delta t^{(n+1)} \dot{\hat{\rho}}_{xy}^{(n+1)} \quad (65)$$

$$f^{(n+1)} = f^{(n)} + \Delta f^{(n)}; \Delta f^{(n)} = \Delta \varepsilon_p^{(n+1)} \partial_{\varepsilon_p} f^{(n)} \quad (66)$$

$$\hat{\rho}_{xy}^{(n=0)} = \hat{\rho}_{xy}; \begin{cases} \mathbf{x} = \mathbf{c}, \mathbf{w}, \mathbf{t}; f^{(n=0)} = f_0. \\ m, i, t \end{cases} \quad (67)$$

For the algorithm to start computing the stress response for the deformation undergone by a specific material point, the yield stress must be calculated first and then substituted in the yield function (Eq. (37)), to check if the material yields. The relations used in the calculation of yield stress can be expressed in the incremental form as follows:

$$\sigma_y^{(n+1)} = \sigma_v^{(n+1)} + \sigma_p^{(n+1)}; \sigma_p^{(n+1)} = \sigma_{pc}^{(n+1)} + \sigma_{pw}^{(n+1)} \quad (68)$$

$$\sigma_{px}^{(n+1)} = Mb(G\tilde{\alpha}_x)^{(n+1)} \sqrt{\rho_0 \rho_{xi}^{(n+1)}}; \mathbf{x} = \mathbf{c}, \mathbf{w}$$

Similarly, from Eqs. (27) and (29),

$$\sigma_v^{(n+1)} = \sigma_{v0}^{(n+1)} \left(\dot{\varepsilon}_p^{(n+1)} \right)^{m_v^{(n+1)}}; \sigma_{v0}^{(n+1)} = \sigma_{v00} [1 + r_v (\hat{T}^{(n)} - 1)^{s_v}];$$

$$\dot{\varepsilon}_p^{(n+1)} \equiv \frac{\dot{\varepsilon}_p^{(n+1)}}{\dot{\varepsilon}_0}; m_v^{(n+1)} = m_{v0} \left[1 + r_v^m (\hat{T}^{(n)} - 1)^{s_v^m} \right] \left(\dot{\varepsilon}_p^{(n+1)} \right)^{m_v^{(n+1)}} \quad (69)$$

The temperature and strain rate dependence are given by the relations in Eq. (35), they are rewritten in incremental forms as follows:

$$C_{xy}^z^{(n+1)} = C_{xy0}^z \left[1 + r_{xy}^z (\hat{T}^{(n)} - 1)^{s_{xy}^z} \right] \left(\dot{\varepsilon}_p^{(n+1)} \right)^{m_{xy}^z};$$

$$m_{xy}^z^{(n+1)} = m_{xy0}^z \left[1 + r_{xy}^m (\hat{T}^{(n)} - 1)^{s_{xy}^m} \right] \quad (70)$$

3.4.4. Stress based return mapping

If the calculated $\phi_{trial}^{(n+1)}$ is greater than zero, the residual functions ($R_i^{(n+1)}$) must be solved using the Newton-Raphson (NR) scheme. The residual functions are obtained from the constitutive relations discussed earlier. The first equation to be solved as a residual function is the yield function itself. This is because the parameters that are obtained from the corrector step should also satisfy the yield function. At the start of the corrector step, the yield function value will be greater than zero indicating that the equivalent stress of the material lies well outside the yield surface, which is not possible, hence the corrector step. At the end of the corrector step, the yield function should become zero as:

$$\phi^{(n+1)} = \left(\frac{\bar{\sigma}^{(n+1)}}{\sigma_y^{(n+1)}} \right)^2 + 2q_1 f^* \cosh \left(\frac{-3q_2 \sigma_h^{(n+1)}}{2\sigma_y^{(n+1)}} \right) - (1 + q_3 f^{*2}) = 0 \quad (71)$$

which can be rewritten in the following form:

$$R_1 = \left(\frac{\bar{\sigma}_{tr}}{1 + 6G \Delta \lambda^{(n+1)}} \right)^2 - \left[1 - 2q_1 f^* \cosh \left(\frac{-3q_2 \sigma_h^{(n+1)}}{2\sigma_y^{(n+1)}} \right) + q_3 f^{*2} \right] \left(\sigma_y^{(n+1)} \right)^2 = 0 \quad (72)$$

The void fraction evolution in Eq. (42) gives the void fraction increment during each time step increment, the equation can be rewritten as:

$$\Delta f = A \Delta \bar{\varepsilon}_p^{(n+1)} + (1 - f^{(n+1)}) \Delta \varepsilon_p^{(n+1)} \quad (73)$$

$$R_2 = f^{(n)} - f^{(n+1)} + A \Delta \bar{\varepsilon}_p^{(n+1)} + 3q_1 q_2 f^* (1 - f^{(n+1)}) \sigma_y^{(n+1)} \Delta \lambda^{(n+1)} \sinh \left(\frac{3q_2 \sigma_h^{(n+1)}}{2\sigma_y^{(n+1)}} \right) \quad (74)$$

The Eq. (47) can be rewritten as:

$$\Delta \bar{\varepsilon}_p^{(n+1)} = \frac{\bar{\sigma}^{(n+1)} \cdot \bar{\varepsilon}_p^{(n+1)} + \sigma_h^{(n+1)} \Delta \varepsilon_p^{(n+1)}}{(1 - f^{(n+1)}) \sigma_y^{(n+1)}} \quad (75)$$

$$\begin{aligned}
R_3 = & 2\Delta\lambda^{(n+1)} \left(\frac{\bar{\sigma}_r}{1 + 6G\Delta\lambda^{(n+1)}} \right)^2 \\
& + 3q_1 q_2 f^* \sigma_y^{(n+1)} \sigma_h^{(n+1)} \Delta\lambda^{(n+1)} \sinh \left(\frac{3q_2 \sigma_h^{(n+1)}}{2\sigma_y^{(n+1)}} \right) \\
& - (1 - f^{(n+1)}) \sigma_y^{(n+1)} \Delta\bar{\epsilon}_p^{(n+1)} \\
= & 0.
\end{aligned} \quad (76)$$

The hydrostatic stress directly influences the damage evolution, and it should also be solved simultaneously, the expression corresponding to it (Eq. (59)) is expanded as follows:

$$\sigma_h^{(n+1)} = \sigma_{trial}^h - K\Delta\epsilon_p^v \quad (77)$$

$$R_4 = \sigma_h^{(n+1)} - \sigma_{trial}^h + 3q_1 q_2 f^* \sigma_y^{(n+1)} K\Delta\lambda^{(n+1)} \sinh \left(\frac{3q_2 \sigma_h^{(n+1)}}{2\sigma_y^{(n+1)}} \right) = 0. \quad (78)$$

The solving scheme is fully integrated i.e., in the initial stages of deformation, the voids formed are very small and hence the flow behavior of the material is dominated by the evolution of dislocation density alone, as the plastic deformation proceeds, the void in the matrix influences the yield function. This whole effect is taken into consideration by coupling the evolution equations of dislocation density, void fractions along with the plastic strain increment and yield function. The residual equations for dislocation densities, which are a part of the fully integrated NR solving scheme. The Eq. (65) is expanded for the different dislocation types as follows:

$$R_5 = \hat{\rho}_{cm}^{(n+1)} - \hat{\rho}_{cm}^{(n)} - \Delta\bar{\epsilon}_p^{(n+1)} \partial_{\epsilon_p} \hat{\rho}_{cm}^{(n)} = 0 \quad (79)$$

$$R_6 = \hat{\rho}_{ci}^{(n+1)} - \hat{\rho}_{ci}^{(n)} - \Delta\bar{\epsilon}_p^{(n+1)} \partial_{\epsilon_p} \hat{\rho}_{ci}^{(n)} = 0 \quad (80)$$

$$R_7 = \hat{\rho}_{wi}^{(n+1)} - \hat{\rho}_{wi}^{(n)} - \Delta\bar{\epsilon}_p^{(n+1)} \partial_{\epsilon_p} \hat{\rho}_{wi}^{(n)} = 0. \quad (81)$$

The residual equations or system of plastic corrector equations are solved simultaneously for every time step increment Δt , trial values are assumed to be start values for $\bar{\sigma}^{(n+1)}$ and $\sigma_h^{(n+1)}$, from the trial stress tensor (Eqs. (52) - (56)), for the state variables ($f^{(n+1)}, \hat{\rho}_{cm}^{(n+1)}, \hat{\rho}_{ci}^{(n+1)}, \hat{\rho}_{wi}^{(n+1)}$), the values from the previous increment step is used as the start values ($f^{(n)}, \hat{\rho}_{cm}^{(n)}, \hat{\rho}_{ci}^{(n)}, \hat{\rho}_{wi}^{(n)}$) and for the plastic multiplier $\Delta\lambda^{(n+1)}$, following calculations are made at the start of corrector step. Using the equation for flow rule (Eq. (44)):

$$\Delta\lambda = \frac{\bar{\sigma}_{trial} \cdot \Delta\bar{\epsilon}_p}{\left(2\bar{\sigma}_{trial}^2 + 3q_1 q_2 f_{trial}^* \sigma_h \sigma_y \sinh \left(\frac{3q_2 \sigma_h}{2\sigma_y} \right) \right)}. \quad (82)$$

The residual functions are combined into a single normalized value as:

$$\hat{R}_{\{k\}}^{(n+1)} = \sqrt{\left(\frac{R_1 \{k\}}{\sigma_y} \right)^2 + \left(\frac{R_2 \{k\}}{\bar{\sigma}_{trial}} \right)^2 + \left(\frac{R_3 \{k\}}{\sigma_{trial}^h} \right)^2 + \left(\frac{R_4 \{k\}}{f^{(n)}} \right)^2 + \left(\frac{R_5 \{k\}}{\hat{\rho}_{cm}^{(n)}} \right)^2 + \left(\frac{R_6 \{k\}}{\hat{\rho}_{ci}^{(n)}} \right)^2 + \left(\frac{R_7 \{k\}}{\hat{\rho}_{wi}^{(n)}} \right)^2} \quad (83)$$

where $\hat{R}_{\{k\}}^{(n+1)}$ is the normalized residual function obtained at the end of $\{k\}^{th}$ iterative step in NR loop index. If the normalized residual function is equal to zero or closer to zero (usually decided if it is lower than certain tolerance value $\chi = 10^{-7}$), the initial values used for the variables are the solution for that time increment step. If the χ value is greater than the tolerance, then initial values are updated iteratively until the solution converges. It is shown as:

$$X_{\{k+1\}}^{(n+1)} = X_{\{k\}}^{(n+1)} - \left(\frac{d\hat{R}_{\{k\}}^{(n+1)}}{dX} \right)^{-1} \hat{R}_{\{k\}}^{(n+1)} \quad (84)$$

where $X_{\{k+1\}}^{(n+1)}$ and $X_{\{k\}}^{(n+1)}$ are vectors comprising values of state variables, constitutive parameters, and plastic strain increment before and after

NR iterative step. $\frac{d\hat{R}_{\{k\}}^{(n+1)}}{dX}$ are the derivatives of every residual function with respect to the variables that are to be solved, which are given as:

$$X^T = [\Delta\bar{\epsilon}_p \quad \Delta\lambda \quad \sigma_h \quad f \quad \hat{\rho}_{cm} \quad \hat{\rho}_{ci} \quad \hat{\rho}_{wi}] \quad (85)$$

$$\frac{d\hat{R}}{dX} = \begin{bmatrix} \frac{\partial R_1}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_1}{\partial \Delta\lambda} & \frac{\partial R_1}{\partial \sigma_h} & \frac{\partial R_1}{\partial f} & \frac{\partial R_1}{\partial \hat{\rho}_{cm}} & \frac{\partial R_1}{\partial \hat{\rho}_{ci}} & \frac{\partial R_1}{\partial \hat{\rho}_{wi}} \\ \frac{\partial R_2}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_2}{\partial \Delta\lambda} & \frac{\partial R_2}{\partial \sigma_h} & \frac{\partial R_2}{\partial f} & \frac{\partial R_2}{\partial \hat{\rho}_{cm}} & \frac{\partial R_2}{\partial \hat{\rho}_{ci}} & \frac{\partial R_2}{\partial \hat{\rho}_{wi}} \\ \frac{\partial R_3}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_3}{\partial \Delta\lambda} & \frac{\partial R_3}{\partial \sigma_h} & \frac{\partial R_3}{\partial f} & \frac{\partial R_3}{\partial \hat{\rho}_{cm}} & \frac{\partial R_3}{\partial \hat{\rho}_{ci}} & \frac{\partial R_3}{\partial \hat{\rho}_{wi}} \\ \frac{\partial R_4}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_4}{\partial \Delta\lambda} & \frac{\partial R_4}{\partial \sigma_h} & \frac{\partial R_4}{\partial f} & \frac{\partial R_4}{\partial \hat{\rho}_{cm}} & \frac{\partial R_4}{\partial \hat{\rho}_{ci}} & \frac{\partial R_4}{\partial \hat{\rho}_{wi}} \\ \frac{\partial R_5}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_5}{\partial \Delta\lambda} & \frac{\partial R_5}{\partial \sigma_h} & \frac{\partial R_5}{\partial f} & \frac{\partial R_5}{\partial \hat{\rho}_{cm}} & \frac{\partial R_5}{\partial \hat{\rho}_{ci}} & \frac{\partial R_5}{\partial \hat{\rho}_{wi}} \\ \frac{\partial R_6}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_6}{\partial \Delta\lambda} & \frac{\partial R_6}{\partial \sigma_h} & \frac{\partial R_6}{\partial f} & \frac{\partial R_6}{\partial \hat{\rho}_{cm}} & \frac{\partial R_6}{\partial \hat{\rho}_{ci}} & \frac{\partial R_6}{\partial \hat{\rho}_{wi}} \\ \frac{\partial R_7}{\partial \Delta\bar{\epsilon}_p} & \frac{\partial R_7}{\partial \Delta\lambda} & \frac{\partial R_7}{\partial \sigma_h} & \frac{\partial R_7}{\partial f} & \frac{\partial R_7}{\partial \hat{\rho}_{cm}} & \frac{\partial R_7}{\partial \hat{\rho}_{ci}} & \frac{\partial R_7}{\partial \hat{\rho}_{wi}} \end{bmatrix} \quad (86)$$

In each iteration, the derivatives specified in the Eqs. (83) - (86) are computed and corrector step is performed (if required). These calculated derivatives are presented in Appendix 1. The stress correction, which is integrated into the radial return algorithm, is encoded as a user-defined material subroutine within ABAQUS Explicit (VUMAT), employing a fully explicit stress-based constitutive integration approach. The schematic representation of this implementation is illustrated in Fig. 3.

4. Material and methods

This section provides a comprehensive analysis of the material's chemical composition and thermo-physical properties, which are essential inputs for the D-TMM model simulations. An in-depth characterization of the undeformed microstructure is conducted to determine the initial dislocation density, serving as a critical input for the model. Additionally, the strategies employed to identify the constitutive and GTN parameters are thoroughly outlined.

4.1. Material and microstructure

S700 is a high strength structural steel with a single-phase microstructure. This steel is used for cold-formed components including cold-pressed parts and sections. Typical applications include steel frames, load bearing beams and pipework. Structures built with high strength steel (HSS) have a high strength to weight ratio and can have longer spans than structures built with mild steel. Nowadays HSS are used in weightlifting applications (e.g., cranes and spreaders), where there is a demand on lightweight design of these structures with increased

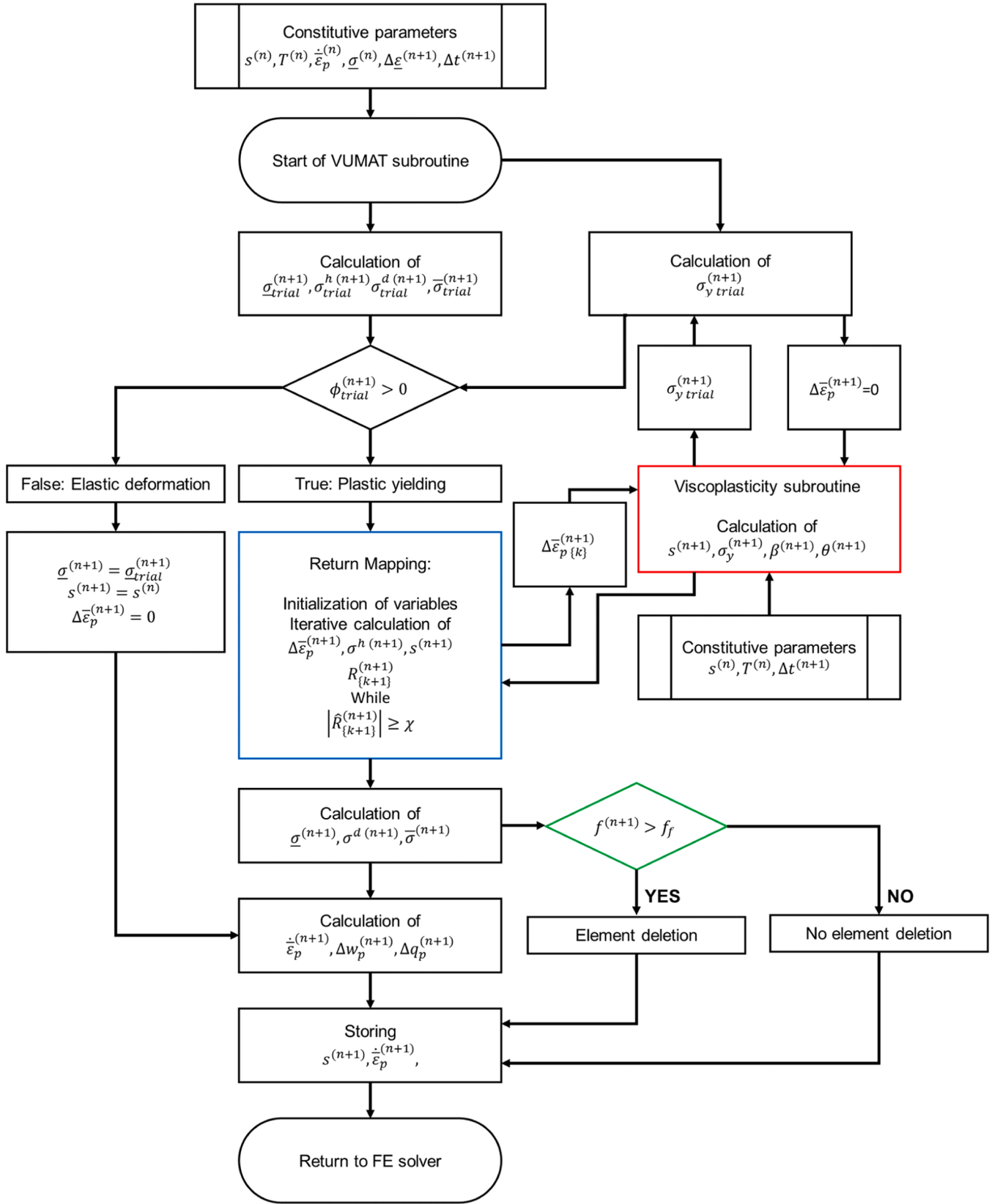
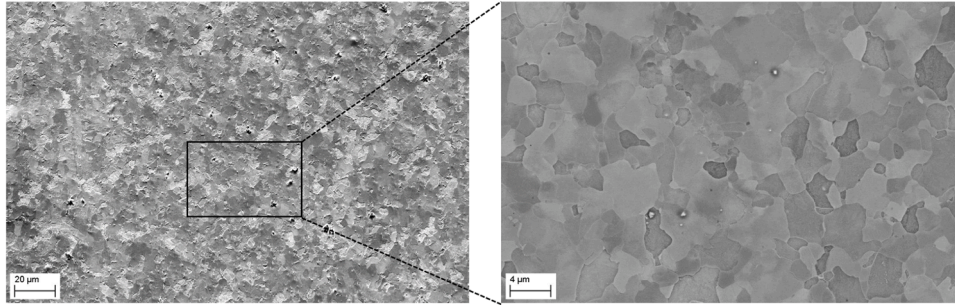


Fig. 3. Flowchart of fully coupled thermo-micro-mechanical model for plasticity and damage behavior of metals (D-TMM). The algorithm is written as a VUMAT subroutine with a viscoplastic material subroutine and return mapping algorithm to calculate material parameters.

Table 2

Chemical composition of the investigated steel S700.

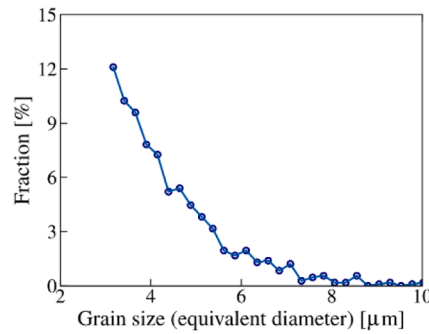
Element	Fe	Mn	Si	Mo	Ti	Al	C	Nb	Cr	Ni	Cu
(wt. %)	96.99	1.921	0.492	0.131	0.126	0.073	0.072	0.048	0.044	0.035	0.024

**Fig. 4.** SEM image of S700 microstructure.

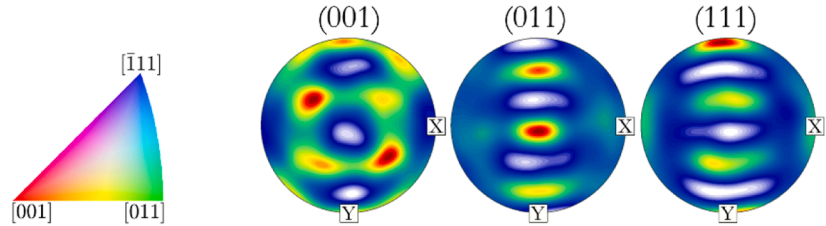
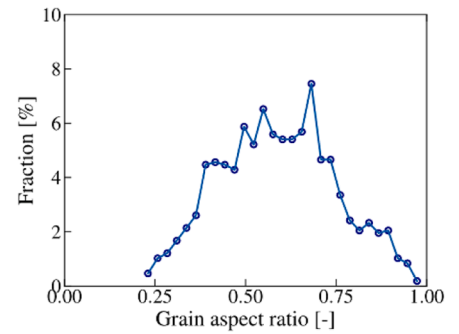
(a) IPF orientation map (undeformed state)



(b) Grain size distribution



(c) Grain aspect ratio distribution



(d) Pole figures calculated from EBSD measurements

Fig. 5. EBSD analysis of the undeformed condition: (a) IPF orientation map, (b) Grain size distribution, (c) Grain aspect ratio distribution, (d) Pole figure.

structural performance [118]. The chemical composition of the S700 was measured using optical emission spectroscopy (OES) as shown in Table 2. The as received fine-grained HSS is alloyed by Mn and Si for solid solution hardening.

The material has a fully ferritic microstructure with equiaxed grains distributed uniformly. There is also presence of some TiC and TiN precipitates, which become evident from SEM investigations and literature. The SEM image of the microstructure is shown in the Fig. 4.

The distribution of the area fractions of grain size and grain aspect ratio based on the EBSD analysis is shown in the Fig. 5 (b) and (c). The inverse pole figure (IPF) and pole figure (PF) for S700 steel in undeformed state is also shown in the Fig. 5(d). From the IPF and PF, the texture of the material can be understood, and it appears to be weakly, almost randomly textured in the undeformed condition.

Thermo-physical properties such as shear modulus, density, thermal expansion co-efficient, specific heat capacity etc. are obtained as a function of temperature for the steel S700 (Fig. 6). The properties were

computed by JMatPro software, based on the chemical composition and temperature range. The respective values are used as an input for thermo-mechanical simulations. In addition to that, the Taylor factor M , Burgers vector b and initial dislocation density ρ for the undeformed state is also determined, as summarized in Table 3.

4.2. Mechanical characterization

In this subsection, we detail the mechanical characterization of as-received S700 single-phase steel sheets, focusing on the preparation and execution of tensile tests to calibrate the constitutive parameters of D-TMM model. The S700 steel sheets, each 2 mm thick, were prepared for tensile testing by waterjet cutting according to ASTM E8 specifications, ensuring a gauge length of 30 mm. To prevent premature failure due to surface defects, the samples were meticulously polished to remove any grooves or imperfections. All specimens were cut in the rolling direction to align with their longest dimension [119].

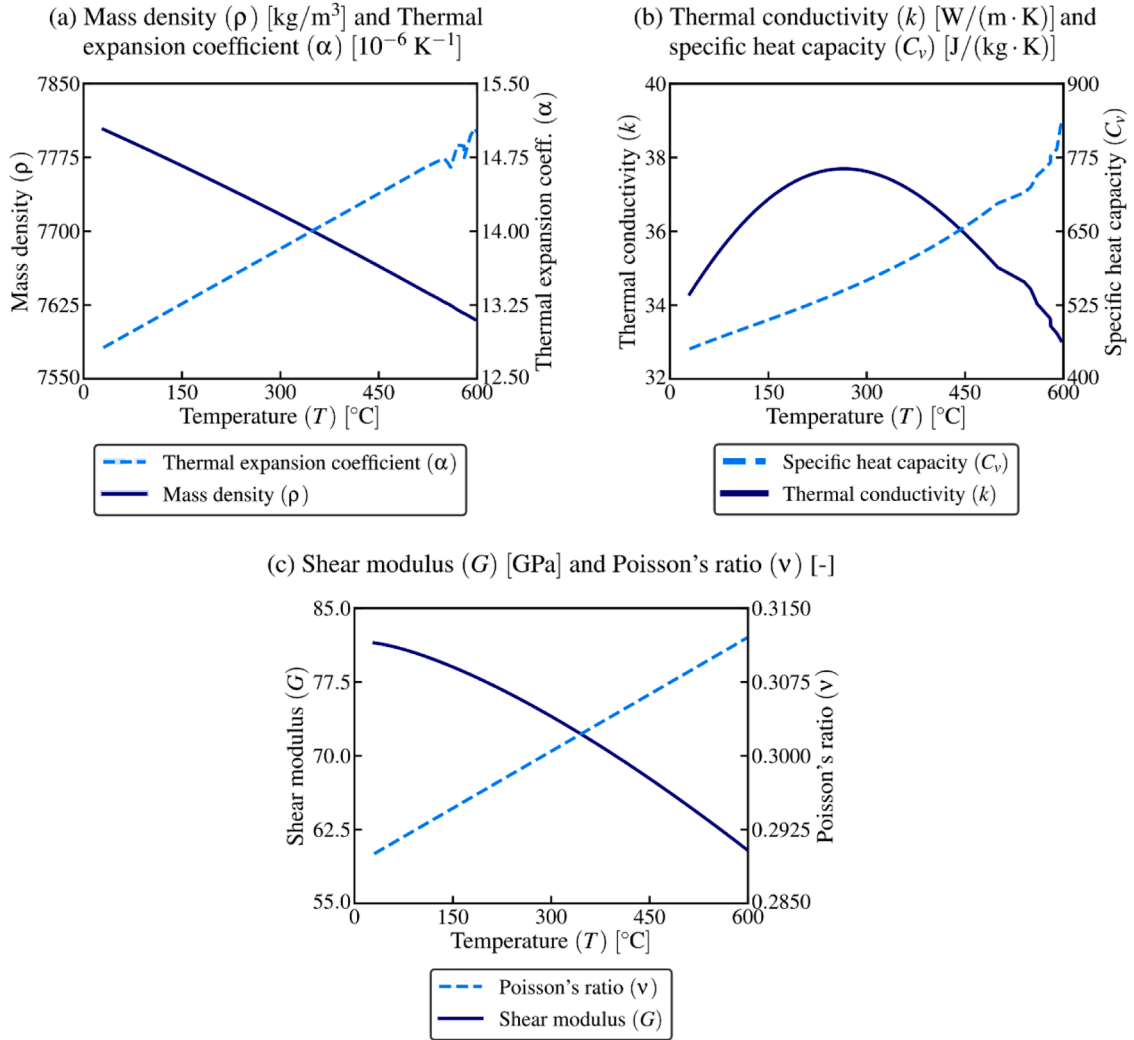


Fig. 6. Thermo-Physical properties of the investigated S700 steel as a function of temperature.

Table 3

Reference parameters and independently measurable required material constants.

T_0 [°C]	$\dot{\epsilon}_0$ [s^{-1}]	ρ_0 [m^{-2}]	M [-]	b [m]
25	0.1	10^{12}	3	2.55×10^{-10}

To fit the constitutive parameters of the models, a series of isothermal tensile tests was conducted. These tests involved uniaxial tensile specimens, notch specimens with various notch radii, and shear specimens at 11 different temperatures (ranging from 25°C to 500°C) and 4 different strain rates (0.0001, 0.001, 0.01, 0.1 s^{-1}). An electro-mechanical universal testing machine, Zwick-Z250 SN, with a maximum force capacity of 250 kN, was employed to execute these tests.

For validation purposes, tensile test samples underwent interrupted testing at a strain rate of 0.1 s^{-1} and a temperature of 25 °C. Interruptions occurred at 1%, 3%, 7%, and 11% plastic strains for plasticity investigations and at 15%, 17%, 19% and 21% for damage mechanism investigations. The deformation zones were then excised, mechanically ground, and polished to a depth of 1 μm before electropolishing. The electropolishing process involved immersing the samples in a solution of 5% perchloric acid and 95% acetic acid, applying a voltage of 31V for 10 seconds. Electron backscatter diffraction (EBSD) analysis was conducted using a Zeiss Sigma SEM instrument with a 75

μm aperture and a field emission gun operated at 20 keV acceleration voltage. Images were captured with a step size of 100 nm over an area of 250 $\mu\text{m} \times 250 \mu\text{m}$. Post-processing of measurement data was performed using the MTEX code implemented in MATLAB. Dislocation density was determined by calculating the kernel average misorientation (KAM) angle, considering grain boundaries with a misorientation greater than 5°. This procedure was replicated for all samples subjected to different strain conditions.

4.3. Identification of constitutive parameters

The results from these tensile tests were utilized to calibrate the model parameters. The D-TMM combines a microstructural model (TMM) for dislocation evolution with the GTN model for damage evolution. Both the evolution of microstructural variables: dislocations and damage—have their own sets of constitutive parameters, defining their evolution behavior based on underlying physics and micromechanical aspects. TMM model parameter identification was carried out in two steps:

1. The first step involves calibrating the constitutive parameters tied to the microstructural model using data from isothermal tensile tests. Engineering stress-strain data collected at different temperatures and strain rates are transformed into plastic stress-strain values. During this phase, only the algorithm governing dislocation density is

- applied, ignoring void effects on plastic response. Plastic response values up to 0.1 strain are used for calibration, as this range is predominantly governed by dislocation evolution alone.
- With the parameters associated with dislocation density identified, the subsequent step determines the damage-related parameters. Engineering stress-strain curves are simulated using the parameters obtained from Step 1, along with initial estimates for the damage parameters. Through an optimization process, the damage parameters are adjusted iteratively until the simulated force curve aligns closely with experimental results, achieving an accurate representation of the material's damage response.

4.3.1. Determination of TMM model parameters

To accurately identify constitutive parameters in Step 1, force curves from uniaxial tensile tests at varying strain rates and temperatures are converted into plastic curves. This calibration process unfolds in two sub-parts, ensuring a precise match with experimental observations across temperature and strain rate variations.

1. Constitutive Parameter Identification at Reference Strain Rate:

The first sub-part addresses parameter calibration for the reference strain rate across a range of temperatures. Here, plastic curves up to a strain of 0.1 are generated and smoothed using a MATLAB 'smooth' algorithm to create stable input curves. These smoothed curves serve as the basis for identifying constitutive parameters, with temperature dependence captured by integrating temperature sensitivity coefficients and exponents into the model. The calibration employs the MATLAB-based FMINCON optimization algorithm, a local minimization solver for constrained multi-variable problems, augmented by suitable global search algorithms to improve robustness. At each iteration, an error function quantifies the difference between calculated and experimental plastic responses, minimizing this error to fine-tune parameter values that will be applicable in finite element simulations.

2. Calibration of Strain Rate Sensitivity via FEMU:

In the second sub-step, the FEMU (Finite Element Model Updating) approach is used to determine strain rate sensitivity parameters and their exponents. Using the constitutive parameters identified in the first sub-part, finite element simulations are conducted for isothermal uniaxial tensile tests at three additional strain rates (0.0001, 0.001, and 0.01 s⁻¹). FEMU is then applied to match the resulting plastic curves with experimental data by adjusting strain rate sensitivity parameters, ensuring the model's fidelity across different strain rates.

Through these two sub-parts, Step 1 ensures that the constitutive parameters are optimized for temperature and strain rate sensitivities, yielding a well-calibrated model for simulating material response under varied loading conditions.

4.3.2. Determination of GTN model parameters

To complete the material model, parameters associated with damage evolution in the GTN model must be accurately determined (according to Step 2 in Section 4.3). The GTN model requires nine key parameters that are divided into three primary categories, each with distinct functions in capturing the material's damage behavior:

1. Empirical Constitutive Parameters:

Parameters q_1 , q_2 and, q_3 are calibrated empirically, with q_3 defined as $q_3 = q_1^2$. Values of $q_1 = 1.5$ and $q_1 = 1.0$ are typical in the literature and serve as standard values for this study, based on findings by Tvergaard [120].

2. Initial Material Parameters:

The initial void fraction f_0 and nucleation parameters f_n and A_N

represent the material's baseline characteristics. These parameters are crucial in defining the onset of void nucleation and growth.

3. Critical Damage Parameters:

The critical void fraction f_c and failure fraction f_f describe the conditions leading to coalescence and failure [121]. The reference value for f_f set at 0.25 as proposed by Tvergaard and Needleman [107], is employed in this study.

To address non-uniqueness in GTN parameter identification, it is essential that parameters derived for various specimen geometries—such as smooth, notched, and center hole specimens—are consistent across loading conditions. To efficiently sample and fit GTN parameters, Latin hypercube sampling (LHS) is employed. LHS ensures a well-distributed sample set across parameter ranges by stratifying the input probability distribution, reducing the total number of samples required while maintaining coverage. A set of 100 initial designs is generated based on the suggested boundaries in

Table 4 and tested using the integrated microstructural material model with damage in isothermal simulations. Force curves and final thickness values of failed specimens from these simulations are compared to experimental data. Simulations with force and thickness values closely matching experimental results are shortlisted for further validation, using simulations on notched samples. This approach helps mitigate non-uniqueness in the parameters by establishing parameter robustness across different geometries and loading scenarios.

4.3.3. Parameter identification strategy for GTN damage parameters

The GTN damage parameters were identified through an optimization process employing two objective functions designed to capture both force and geometric consistency between simulation and experimental results. Using the force curves and specimen widths derived from LHS designs, the coupled D-TMM model for finite element (FE) simulations was calibrated against the experimental outcomes from uniaxial tensile tests. The two objective functions were evaluated at specific intervals to enhance the reliability of parameter fitting.

- Objective Function (OBJ 1): This objective function directly compares the simulated and experimental force values at predefined displacement intervals, ensuring the model accurately replicates the material's load-bearing response. The objective equation is given as:

$$OBJ1 = \sum_{k=1}^k (F_k - F'_k)^2, \quad (87)$$

where k represents the number of displacement points at which force values are compared, F_k is the experimentally measured force, and F'_k is the simulated force at the k^{th} displacement point.

- Objective Function (OBJ 2): Based on the methodology in [122], this function focuses on the specimen's width at failure, addressing the non-uniqueness issue by adding a geometric constraint. This function compares widths across different cross-sections between the simulated and experimental results, helping ensure that the model

Table 4

The lower, center, and upper bounds for Latin hypercube sampling method.

Parameter	Reference	Minimum	Maximum
f_0	0.0006	0.0001	0.001
f_n	0.125	0.001	0.05
f_c	0.07	0.01	0.1
f_f	0.25	0.1	0.3
q_1	1.5	1	2
q_2	1.0	0.5	1.5
e_N	0.2	0.1	0.3

accurately predicts deformation patterns beyond just load response. It is expressed as:

$$OBJ2 = \sum_{j=1}^j (d_j - \hat{d}_j)^2, \quad (88)$$

where j represents specific cross-section positions along the specimen during failure, d_j is the experimentally measured width, and $\hat{d}_j$ is the simulated width at position j .

The combined overarching objective function (OBJ) integrates both force and geometric considerations, providing a balanced approach to parameter optimization that addresses the GTN model's sensitivity to both loading and structural deformation aspects:

$$OBJ = \frac{OBJ1 + OBJ2}{2}. \quad (89)$$

Minimizing this composite function yields an optimized set of GTN damage parameters specifically calibrated for S700 steel, ensuring that both load-bearing and structural deformation responses align closely with experimental data. This dual-objective approach enhances model accuracy, addressing both material behavior underload and the integrity of structural predictions through failure.

4.4. Model for FE simulations

This section outlines the development and implementation of the finite element (FE) model used to simulate isothermal tensile tests, with the aim of determining the strain rate sensitivity parameters and calibrating the GTN damage parameters. A tailored VUMAT/Explicit subroutine was created to integrate the D-TMM within the Abaqus/Explicit environment. This setup was specifically structured to reflect the exact dimensions of the specimens used in physical testing, ensuring accurate comparison with experimental results.

Given the thermally coupled nature of the material model, simulations were conducted in a dynamic, temperature-dependent framework using C3D8RT elements, which are 8-node thermally coupled brick elements suitable for explicit analysis. Prior to initiating the simulations, mesh sensitivity and mass scaling analyses were performed. Through these analyses, an optimal mesh density of 0.25mm and a mass scaling factor of 10^3 were established, balancing computational efficiency and accuracy in capturing the material behavior during deformation.

The accuracy and reliability of these FE simulations were validated by comparing the constitutive parameters against those obtained from the RMVA (RMV based Analysis) method for the reference strain rate. This validation was crucial to confirm the model's capability to consistently replicate experimental conditions and predict accurate material responses.

Upon determining the strain rate sensitivity parameters through FEMU methods (Section 4.3.1), the constitutive model was updated with the identified parameters, and the same FE simulations were applied to address the GTN damage parameters (Section 4.3.3). Thus, the developed FE model provides a robust framework for evaluating and updating constitutive and damage parameters in the D-TMM model, ensuring it can accurately represent the complex interplay of strain rate, temperature, and damage evolution under isothermal tensile conditions.

5. Results, discussions and validations

To evaluate the performance of the D-TMM model, FE simulations were conducted under both isothermal and non-isothermal conditions across various temperatures. The model's predictions were validated against experimental data, focusing on key microstructural features such as GND density evolution and damage mechanisms. This validation involved comparing the model's outputs with experimental

characterizations obtained under identical conditions. The comprehensive assessment provided insights into the distribution and evolution of MSVs, including dislocation densities and void fractions, as well as the macroscopic stress-strain responses. This section outlines the detailed findings, emphasizing the correlation between predicted and experimentally observed microstructural features and macroscopic properties, highlighting the strengths and limitations of the D-TMM model.

5.1. Constitutive parameters of plasticity model

The D-TMM model's constitutive parameters are determined through meticulous analysis of flow stress data from isothermal tensile tests conducted at various strain rates and temperatures (Section 4.3). To focus on the material's plastic behavior, stress-strain curves are processed to minimize noise, producing smooth plastic curves up to a strain of 0.1, beyond which damage effects become significant. Only the undamaged portions of these curves are utilized for calibrating plastic model parameters (Section 4.3.1). To gain insights into the evolution of dislocation density, interrupted tensile tests are performed at incremental strain levels. Post deformation, specimens are prepared for microstructural analysis. High-resolution EBSD is employed to measure GND densities within the deformed regions (Section 4.2), providing a basis for validating the model's microstructural predictions.

The reference conditions for the experiments, detailed in Table 3, which has room temperature as the baseline temperature T_0 and a strain rate of $0.1s^{-1}$ as the reference strain rate $\dot{\epsilon}_0$. Tests are conducted up to 500 °C to limit the influence of recrystallization. The experiments span the quasi-static range ($10^{-4}s^{-1} - 10^{-1}s^{-1}$) and a temperature range of 25 °C to 500 °C. As outlined in the parameter identification (Section 4.3.1), constitutive parameters are determined using the RMVA approach. The parameter calibration process involves minimizing the error function to ensure close alignment between model-predicted dislocation evolution and experimentally derived values from EBSD analysis. The finalized set of constitutive parameters, validated for the material response at the reference state, is provided in Table 5. Temperature-related effects on material response are accounted for through temperature sensitivity coefficients and exponents, detailed in Table 6, which adjust the parameters to reflect changes with increasing temperature. Constitutive parameters identified in the second step of calibration procedure by FEMU technique using uniaxial tensile tests at different strain rates to account for the effect of strain rate related effects are presented in Table 7.

5.1.1. Discussions: Temperature dependencies on dynamic dislocation processes

This section examines the dislocation dynamics in S700 steel, focusing on the probability amplitudes of various dislocation processes across different temperature ranges that are determined in Section 5.1. Fig. 7 (a-g) illustrates the temperature dependence of the dynamic dislocation processes, derived from constitutive parameters and temperature-dependent coefficients in Tables 5 and 6. We consider three temperature regimes for analysis: the "cold regime" ($0^\circ\text{C} < T \leq 150^\circ\text{C}$), an intermediate range ($200^\circ\text{C} \leq T \leq 300^\circ\text{C}$), and the "warm regime" ($350^\circ\text{C} \leq T < 500^\circ\text{C}$).

Dynamic annihilation and remobilization processes, collectively termed dynamic recovery, are primarily governed by dislocation climb and cross-slip mechanisms [123,124]. At lower temperatures, these processes are driven by cross-slip, a mechanism that allows dislocations to move across slip planes. With increasing temperature, dislocation climb, a diffusion-controlled process enabled by vacancy movement, becomes more significant [125,126]. Additional remobilization can occur due to junction dissociation and bow-out [79], both of which increase dislocation mobility, while mutual annihilation involves the interaction of a mobile dislocation with another dislocation, either mobile or immobile, and can proceed via cross-slip (for screw dislocations) or climb (for edge dislocations) [81,123].

Table 5

Initial cell mobile, cell immobile and wall immobile dislocations; viscous stress at reference conditions; constitutive parameters associated with probability amplitude of different dislocation processes, mean interaction strengths for S700 steel.

$c_{cm}^{an} [-]$	$c_{cm0}^{an} [-]$	$c_{ci0}^{an} [-]$	$c_{wi0}^{an} [-]$	$c_{ci}^{ac} [-]$	$c_{wi}^{ac} [-]$	$c_{cm0}^{tr} [-]$	$c_{wi0}^{nc} [-]$
2877.23	0.06004	0.09873	0.00984	8.20196	1.13865	1.60547	0.02423
$c_{ci0}^{rm} [-]$	$c_{wi0}^{rm} [-]$	$\tilde{\alpha}_{c0} [-]$	$\tilde{\alpha}_{w0} [-]$	$\hat{\rho}_{cm0} [-]$	$\hat{\rho}_{ci0} [-]$	$\hat{\rho}_{wi0} [-]$	$\sigma_{v00} [MPa]$
11.049	0.02244	0.09901	0.31634	76.5583	228.333	342.86	270.124

Table 6

Temperature sensitivity coefficients and exponents for constitutive parameters and viscous stress for S700 steel.

$r_{cm}^{an} [-]$	$r_{ci}^{an} [-]$	$r_{wi}^{an} [-]$	$r_{cm}^{tr} [-]$	$r_{wi}^{nc} [-]$	$r_{ci}^{rm} [-]$	$r_{wi}^{rm} [-]$	$r_{ac}^G [-]$	$r_{aw}^G [-]$	$r_v [-]$
0.1744	0.654	1.2717	8.2286	0.7945	4.4965	4.5664	-0.6233	-0.0505	-1.9223
$s_{cm}^{an} [-]$	$s_{ci}^{an} [-]$	$s_{wi}^{an} [-]$	$s_{cm}^{tr} [-]$	$s_{wi}^{nc} [-]$	$s_{ci}^{rm} [-]$	$s_{wi}^{rm} [-]$	$s_{ac}^G [-]$	$s_{aw}^G [-]$	$s_v [-]$
4.0456	0.9959	1.4155	1.5952	3.9165	2.4535	8.0155	0.2449	1.2553	0.9363

Table 7

Constitutive parameters (strain rate sensitivity) identified by FEMU method.

$m_{v0} [-]$	$r_v^m [-]$	$s_v^m [-]$	$m_v^m [-]$	$\kappa [-]$
2877.23	0.06004	0.09873	0.00984	8.20196

In the "cold regime," Fig. 7 (a-c) and Fig. 7 (f-g) shows that dynamic annihilation of cell mobile dislocations remains relatively unaffected by temperature. Meanwhile, annihilation behavior of cell immobile and wall immobile dislocations exhibit a more linear response to temperature, suggesting a gradual increase due to thermal activation. Remobilization is minimal in this range, indicating that cross-slip, rather than climb, is the dominant mechanism. As temperature increases into the "warm regime," recovery mechanisms shift towards dislocation climb due to increased thermal activation and vacancy diffusion. This is evident from Fig. 7 (a-c), which reveals a rapid increase in the amplitude of annihilation for mobile dislocations and a slight increase for wall immobile dislocations. The lower energy threshold required for climb enables significant remobilization, which is crucial to material recovery at high temperatures [81,127]. This shift is also evident in Fig. 7 (f-g), where remobilization amplitudes for cell immobile dislocations increase substantially, creating mobile dislocations that further drive annihilation. At elevated temperatures, even stable boundaries begin to remobilize, promoting material softening and reducing creep resistance. Higher remobilization amplitudes for cell immobile dislocations suggest their instability at increased temperatures, favoring dislocation wall formation. Enhanced remobilization reflects reduced lattice friction and greater dislocation mobility, which are characteristics of high-temperature deformation.

Fig. 7 (d) reveals an increase in cell mobile dislocation trapping at higher temperatures, attributed to interactions with dislocations on intersecting slip systems, forming Lomer-Cottrell locks or stable junctions [91,93,94]. Elevated temperatures increase cell mobile dislocation availability due to remobilization and solute diffusion, enabling interstitial atoms to pin them at junctions [96,128]. Despite ongoing remobilization, some of these trapped dislocations achieve sufficient stability to create localized stress concentrations, promoting the alignment of dislocations into walls [129], as indicated by the increased wall nucleation amplitude in Fig. 7 (e). Wall nucleation suggests a transition to organized substructures driven by local stress fields and dislocation gradients. This critical phase in the thermal evolution of S700 steel's microstructure reflects increased dislocation mobility and boundary stabilization at high temperatures, contributing to material softening.

In summary, the dislocation dynamics in S700 steel demonstrate a transition from low-temperature cross-slip mechanisms to high-temperature climb-dominated processes, with remobilization and wall formation becoming increasingly significant. This shift highlights the effect of thermal activation on dislocation behavior, influencing

mechanical properties by promoting recovery, reducing strength, and impacting creep resistance at elevated temperatures.

Fig. 8 illustrates the thermal sensitivity of key dislocation-based strengthening mechanisms ($G\tilde{\alpha}_c$ & $G\tilde{\alpha}_w$), viscous stress σ_v , and strain rate sensitivity m_v in S700 steel. As temperature rises, a decrease in shear modulus occurs (Fig. 6), primarily due to thermal expansion and reduced lattice stability, which diminishes the material's resistance to dislocation motion. This reduction in shear modulus weakens the dislocation interaction strength (Fig. 8a and b), meaning that dislocation barriers such as cell and wall dislocations become less effective. Consequently, S700 steel exhibits reduced resistance to dislocation movement at higher temperatures, signaling a trend toward easier plastic flow and impacting its mechanical properties in high-temperature environments.

The decline in viscous stress with increasing temperature aligns with the expected thermal activation of dislocation movement processes, such as climb and cross-slip. These mechanisms facilitate dislocation motion more readily at elevated temperatures, implying that S700 steel becomes more deformable, with lower resistance to dislocation motion as temperature increases. In contrast, strain rate sensitivity, reflecting the change in flow stress relative to strain rate, increases with temperature. This trend suggests a shift from rate-insensitive behavior at low temperatures to a more ductile, rate-sensitive response at higher temperatures.

The decreasing values of dislocation interaction coefficients ($G\tilde{\alpha}_c$ & $G\tilde{\alpha}_w$), and viscous stress σ_v indicate a clear softening effect, underscoring the material's temperature-dependent strength. The increase in strain rate sensitivity m_v at elevated temperatures further supports this softening, pointing to improved ductility and reduced brittleness in S700 steel as it transitions to higher temperatures.

5.2. Isothermal uniaxial tests

Isothermal uniaxial tensile tests were conducted as outlined in Section 4.2 to obtain experimental flow curves for S700 steel. Using the constitutive parameters determined in Section 5.1 and the uniaxial tensile test FE simulation model from Section 4.4, simulated flow curves were generated under identical conditions and compared with experimental results, as shown in Fig. 9. The close alignment of the experimental and simulated curves indicates effective model calibration. Notably, these simulations extend only up to 0.1 plastic strain, as plasticity dominates within this range, while damage mechanisms play an increasingly significant role beyond this threshold. For analysis, temperature ranges were divided into the "cold regime" ($0^\circ\text{C} < T \leq 150^\circ\text{C}$), intermediate range ($200^\circ\text{C} \leq T \leq 300^\circ\text{C}$), and "warm regime" ($350^\circ\text{C} \leq T < 500^\circ\text{C}$), as discussed in Section 5.1.1.

The temperature dependence of dislocation dynamics, as outlined in Section 5.1.1, drives the macroscopic flow behavior through their

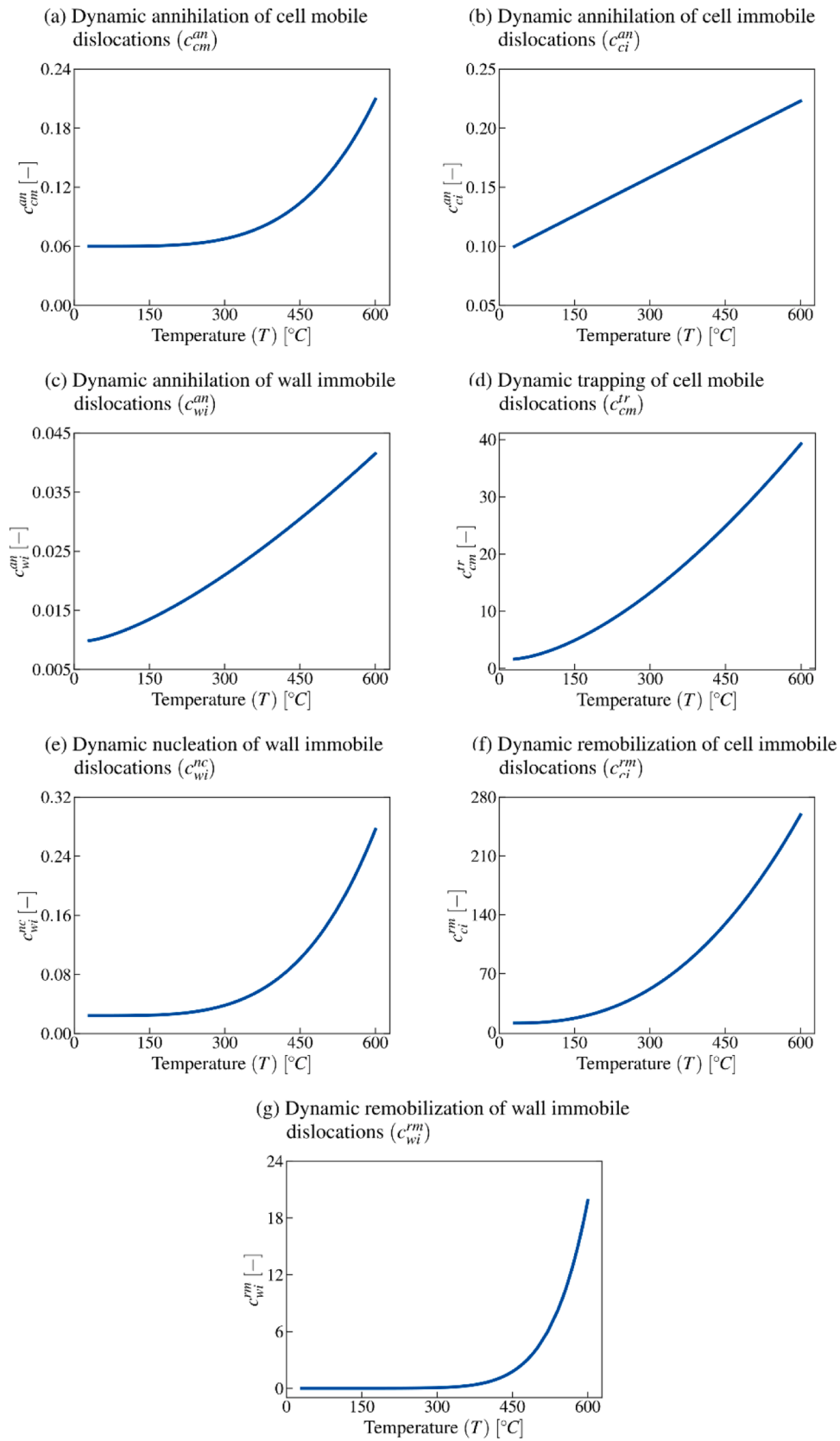


Fig. 7. Temperature dependencies of probability amplitudes of different thermal dynamic dislocation processes.

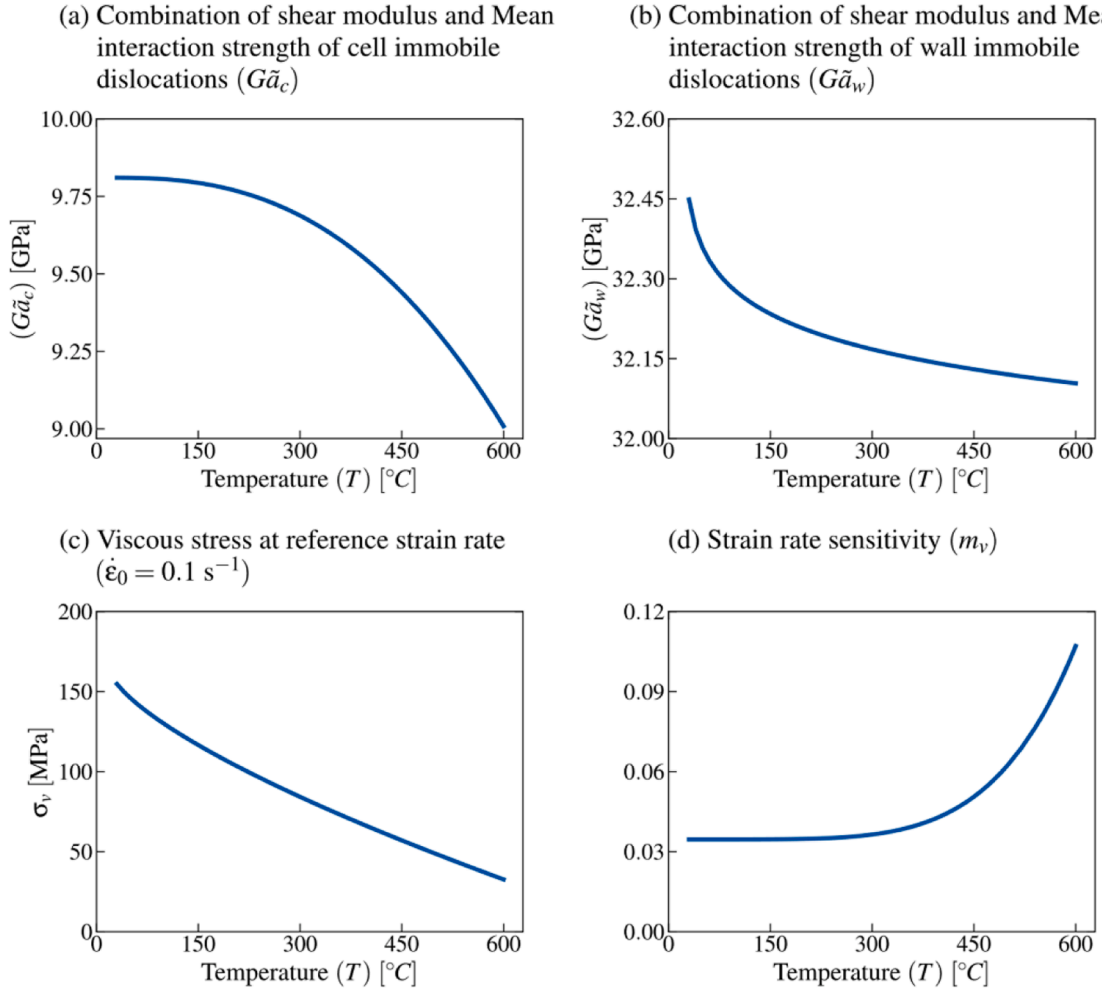


Fig. 8. Temperature dependence of combination of shear modulus, mean interaction strength, viscous stress, and strain rate sensitivity.

interactions because of temperature and deformation. This dependence can be interpreted as resulting from two opposing processes: dynamic thermal softening (DTS) and dynamic thermal hardening (DTH). DTS primarily arises from increased dynamic annihilation and remobilization of cell immobile dislocations, along with reductions in viscous stress and dislocation interaction contributions as temperature rises. In contrast, DTH results from dynamic strain aging due to the pinning of cell mobile dislocations by interstitial atoms like C and N, alongside the dynamic nucleation of wall immobile dislocations.

5.2.1. Discussions on strength and ductility metrics of S700 steel

The interplay between DTS and DTH mechanisms is evident in the material's strength and ductility metrics based on the experimental investigations. Key metrics, including hardening capacity, yield stress, and the yield-to-tensile (Y/T) ratio, help elucidate the influence of competing dislocation mechanisms on the macro scale across temperature ranges.

Yield stress (σ_{y0}): A key strength metric, yield stress indicates the material's initial resistance to deformation.

Hardening capacity (C): This metric assesses a material's ability to strengthen with continued deformation, calculated as:

$$C = \frac{\sigma_s - \sigma_{y0}}{\sigma_s} = 1 - \frac{\sigma_{y0}}{\sigma_s}, \quad (90)$$

where σ_s represents the saturated yield stress.

Yield-to-tensile ratio (S): A measure of a material's ductility and deformation capacity and capacity to absorb energy before failure, with

lower ratios reflecting greater ductility. It is defined as:

$$S = \frac{\sigma_{y0}}{\sigma_{ut}}, \quad (91)$$

where σ_{ut} is the ultimate tensile strength.

Fig. 10c illustrates the temperature-dependent yield stress for S700. In the cold regime, DTS dominates, leading to a decrease in yield stress, primarily due to reduced viscous stress contributions, as seen in Fig. 8c. This effect extends to the flow curves in cold regime (Fig. 9a), where flow curves near the intermediate temperature range starts to converge, indicating an emerging influence of DTH. As temperatures rise into the intermediate range, DTH effects strengthen due to increased dynamic trapping of cell mobile dislocations and nucleation of wall immobile dislocations (Fig. 7d and e). This shift raises the yield stress with temperature (Fig. 10c), also influencing the flow curves in Fig. 9b. In the warm regime, as shown in Fig. 7 (a-c) and (f-g), the amplitudes for dynamic annihilation and remobilization of cell immobile and wall immobile dislocations significantly increase, leading to a pronounced DTS effect that surpasses DTH. Consequently, both flow curves (Fig. 9c) and yield stress (Fig. 10c) exhibit a downward trend in this range, underscoring the dominance of DTS and the resulting reduction in material strength at elevated temperatures.

In cold regime (Fig. 10), the hardening capacity (C) remains moderate, and the yield-to-tensile ratio (S) is high, reflecting low ductility exhibited by S700 steel at low temperatures. In this range, DTS effects are limited, with dislocations pinning contributing DTH, which aids in hardening. In the intermediate range, DTH effects intensify, leading to

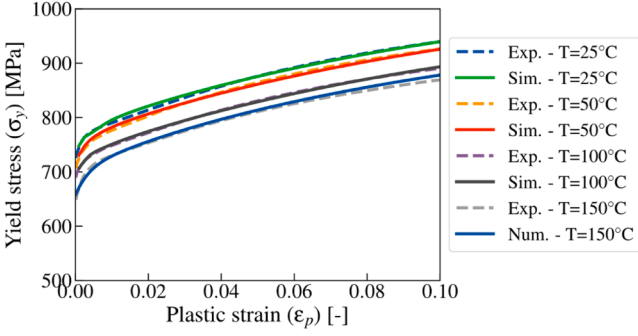
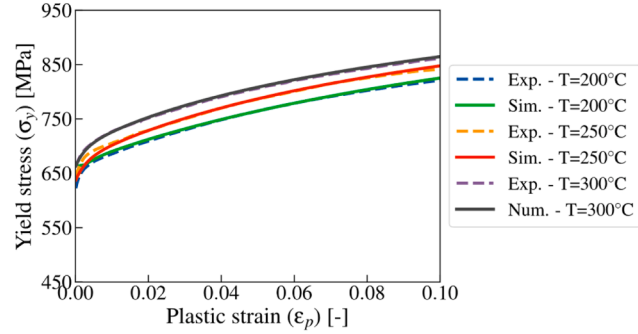
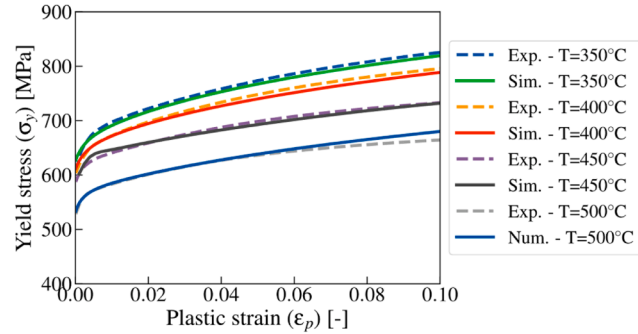
(a) Cold Temperatures ($0^{\circ}\text{C} < T < 200^{\circ}\text{C}$)(b) Intermediate Temperatures ($200^{\circ}\text{C} \leq T < 350^{\circ}\text{C}$)(c) Warm Temperatures ($350^{\circ}\text{C} \leq T \leq 500^{\circ}\text{C}$)

Fig. 9. Comparison between experimental and computational flow curves at different temperatures (isothermal condition) for tensile tests at reference strain rate ($\dot{\epsilon}_0 = 0.1\text{s}^{-1}$).

increased hardening capacity and yield-to-tensile ratio, where dynamic strain ageing (DSA) occurs as interstitial atoms pin mobile dislocations, this hardening strengthens the material but reduces its ductility. At warmer regimes, DTS becomes dominant, resulting in substantial dislocation annihilation and remobilization, reducing dislocation density and softening the material. This softening lowers the hardening capacity and yield-to-tensile ratio, enhancing ductility but reducing strength. Thus, across temperature ranges, the balance between DTS and DTH mechanisms in S700 steel directly affects its strength and ductility, with higher temperatures favoring softening and increased ductility.

5.2.2. FE simulations of plastic deformation in S700 steel using D-TMM model

The presented constitutive model has been implemented as a user-defined material subroutine (VUMAT) in ABAQUS/Explicit, utilizing material parameters identified during the RMV-based fitting process outlined in Section 4.3.1. A thermo-mechanical finite element (FE) model of the uniaxial tensile test was developed in ABAQUS/Standard,

incorporating the nominal dimensions of the experimental specimens and testing apparatus.

To ensure accurate representation of material behavior, the mechanical and physical properties of both the material and testing tools, such as elastic modulus, Poisson's ratio, mass density, specific heat capacity, thermal conductivity, and thermal expansion, were defined as temperature-dependent inputs in the FE model. This comprehensive setup facilitates the simulation of both mechanical and thermal interactions during deformation, enabling precise evaluation of the material's response under various loading and thermal conditions.

At a plastic strain of 0.1, the FE simulation results (Fig. 11) reveal key insights into the distribution of equivalent stress, dislocation densities, plastic strain, and void fractions in S700 steel. The uniform deformation observed along the gauge length, indicated by the homogeneous distribution of equivalent stress and strain, confirms that the material response at this stage is dominated by plastic deformation mechanisms. Notably, the absence of localized void concentration suggests that damage mechanisms have not yet become significant, as the void fractions remain evenly distributed.

These simulations were instrumental in generating the flow curves presented in Fig. 9, demonstrating the model's ability to predict macroscopic behavior. Additionally, the results provide a preliminary understanding of the interplay between macroscopic responses—such as stress and strain—and the evolution of microstructural state variables, including dislocation densities and void fractions, offering a foundation for correlating material behavior across different scales.

5.3. Evolution of dislocation density at reference conditions

The evolution of dislocation densities in S700 steel under isothermal conditions at various temperatures and a reference strain rate is depicted in Fig. 12. The figures present the progression of (a) cell mobile, (b) cell immobile, (c) wall immobile, and (d) total dislocation densities.

Initially, at low strain levels, cell mobile dislocations ρ_{cm} (Fig. 13a) show a high density, which rapidly decreases with increasing strain, reflecting dynamic annihilation processes. This reduction in mobile dislocation density is more pronounced at intermediate ($200^{\circ}\text{C} \leq T \leq 300^{\circ}\text{C}$) and higher ($350^{\circ}\text{C} \leq T < 500^{\circ}\text{C}$) temperatures, where thermally activated recovery mechanisms, particularly dislocation climb, accelerate the annihilation of mobile dislocations. For cell immobile dislocations ρ_{ci} (Fig. 13b), density initially increases with strain, reaching a peak before beginning to decline, especially noticeable at lower temperatures ($0^{\circ}\text{C} < T \leq 150^{\circ}\text{C}$). At higher temperatures, this peak occurs at a lower strain and has a diminished intensity due to enhanced remobilization and recovery effects. This behavior aligns with the transition from cross-slip-dominated mechanisms at low temperatures to climb-facilitated annihilation and increased dislocation mobility at higher temperatures. Wall immobile dislocation density ρ_{wi} (Fig. 13c) shows a consistent increase with strain across all temperatures; however, the rate of accumulation slows down as temperature rises. This suggests that while dislocation walls stabilize under localized stress fields at higher strains, thermal effects, particularly at higher temperatures, promote boundary remobilization. Even with climb mechanisms aiding remobilization, wall dislocations persist as effective barriers, leading to a gradual but continual accumulation at elevated temperatures.

The overall or total dislocation density ρ_{tot} (Fig. 13d) rises with strain but with a moderated rate of increase at higher temperatures. This tempered rise can be attributed to temperature-activated recovery mechanisms—such as cross-slip and climb—that collectively limit dislocation buildup. Consequently, the softening effects due to reduced lattice friction and increased dislocation mobility become dominant at higher temperatures, where recovery processes effectively balance or reduce dislocation accumulation as plastic deformation progresses. This behavior highlights the critical role of temperature-dependent mechanisms in dislocation evolution and their influence on the material's hardening and softening responses under strain.

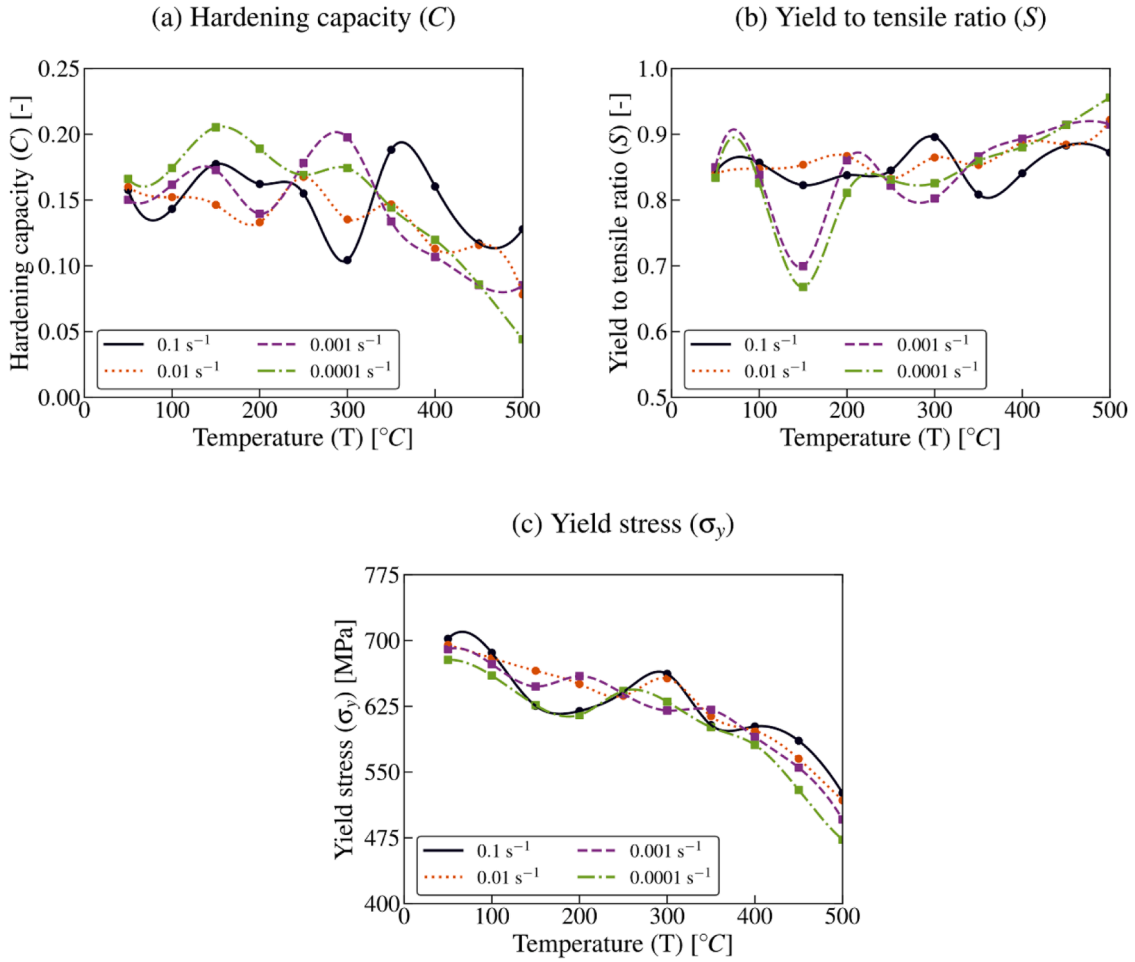


Fig. 10. Strength and ductility metrics with respect to temperature for various strain rates in the quasi-static range and temperatures for S700 steel.

5.4. GND density measurements – Validation for D-TMM model predictions

To ensure the accuracy of the constitutive parameters determined in Section 5.1 through the RMVA approach, a validation step is conducted by comparing the dislocation densities predicted by the material model, using material parameters from Section 5.1, with experimentally obtained dislocation density values from isothermal uniaxial testing under reference conditions. This comparison is essential for assessing the model's capability to predict microstructural evolution accurately, confirming whether the calibrated parameters capture the underlying dislocation dynamics effectively.

The GND density is experimentally measured by interrupting tensile test samples at incremental plastic strains, specifically at 1%, 3%, 7%, and 11%. These strain values are chosen to remain within the plasticity-dominated region ($\epsilon_p \leq 0.1$), allowing for a focused analysis in the absence of significant damage effects. EBSD measurements are performed on these interrupted samples, with detailed descriptions of the sample preparation and measurement process provided in Section 4.2. To ensure consistency, the measurement location is selected from the center of the tensile specimen, as illustrated in Fig. 13(a), where the local equivalent plastic strain is close to the mean equivalent plastic strain. The same location is carefully matched in the FE simulation model. Initial reference measurements on the undeformed sample, with dislocation distribution highlighted in yellow, are shown in Fig. 13(b). At each strain increment, the GND density is derived from the kernel average misorientation (KAM) angle, a measurement from EBSD that reflects the angular deviation between two points with a misorientation

below 5°. These KAM values are then mapped to GND density, then average GND density for the representative area is calculated. The EBSD measurements for increasing strains, displayed in Fig. 13 (d-g), demonstrate a clear correlation between strain increase and dislocation density rise.

For comparison with simulation results, the model-predicted wall dislocation density ρ_{wi} is used, as this component is modelled to arise from misorientations due to lattice torsion, warp, or twist. This comparison, presented in Fig. 13 (c), provides a validation of the model's capability to simulate the wall dislocation density and align with experimentally observed GND densities.

5.5. Constitutive parameters of GTN damage model

The temperature- and deformation-dependent constitutive parameters for S700 steel (In Section 5.1), derived based on dislocation dynamics, have been determined and experimentally validated for conditions dominated by plastic deformation (Section 5.4). This validation is applicable up to the onset of damage mechanisms. To capture the influence of damage, the GTN model has been integrated with the isotropic hardening framework as detailed in Section 3.4. This integration enables the D-TMM model to incorporate void fraction evolution alongside dislocation evolution, capturing the complex interactions necessary to describe the material's yield behavior accurately. The GTN damage parameters, determined through the calibration process described in Section 4.3, are listed in Table 8.

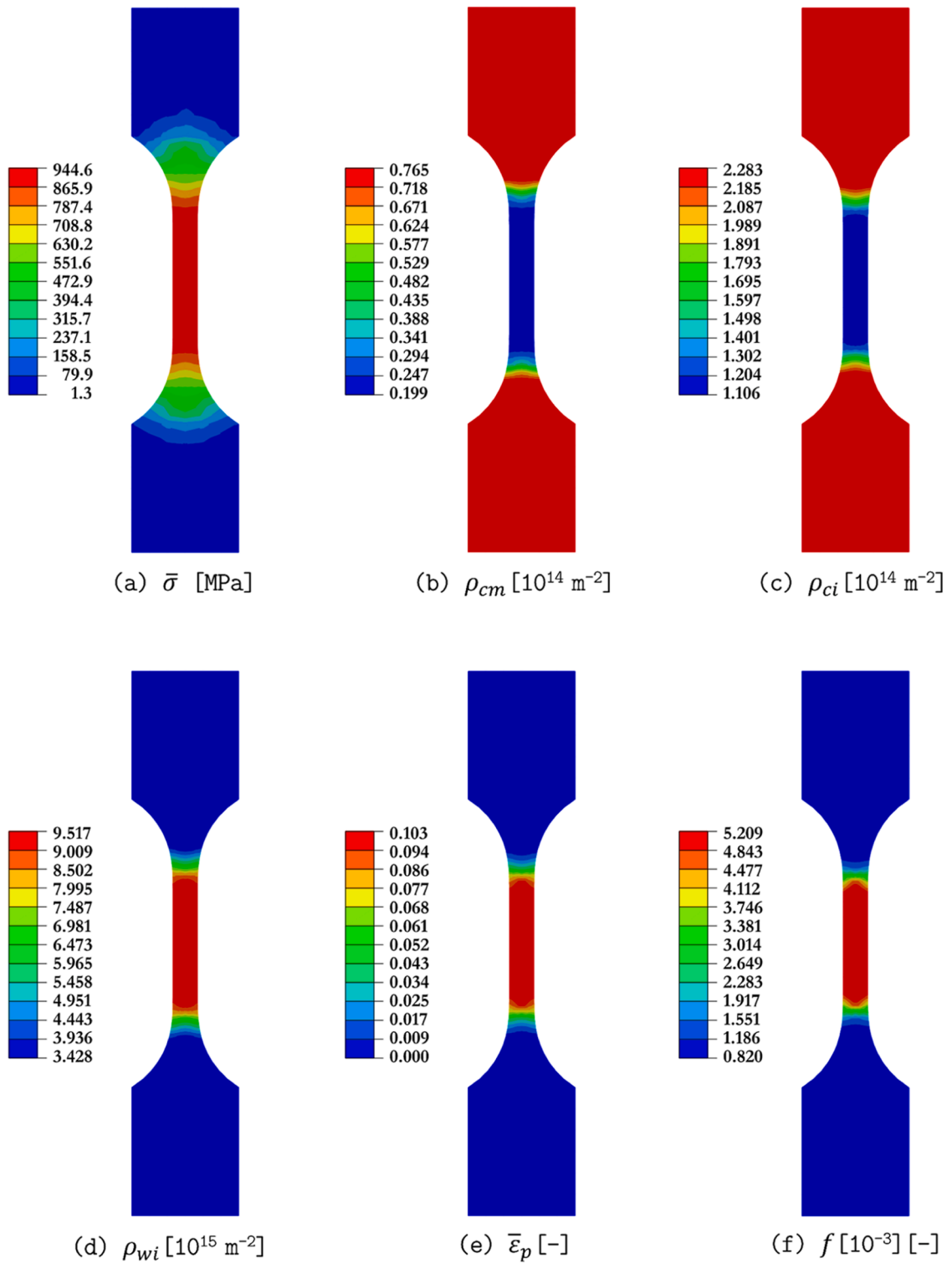


Fig. 11. Results from FE simulation of isothermal tensile test in the plasticity dominated regime using the D-TMM material model.

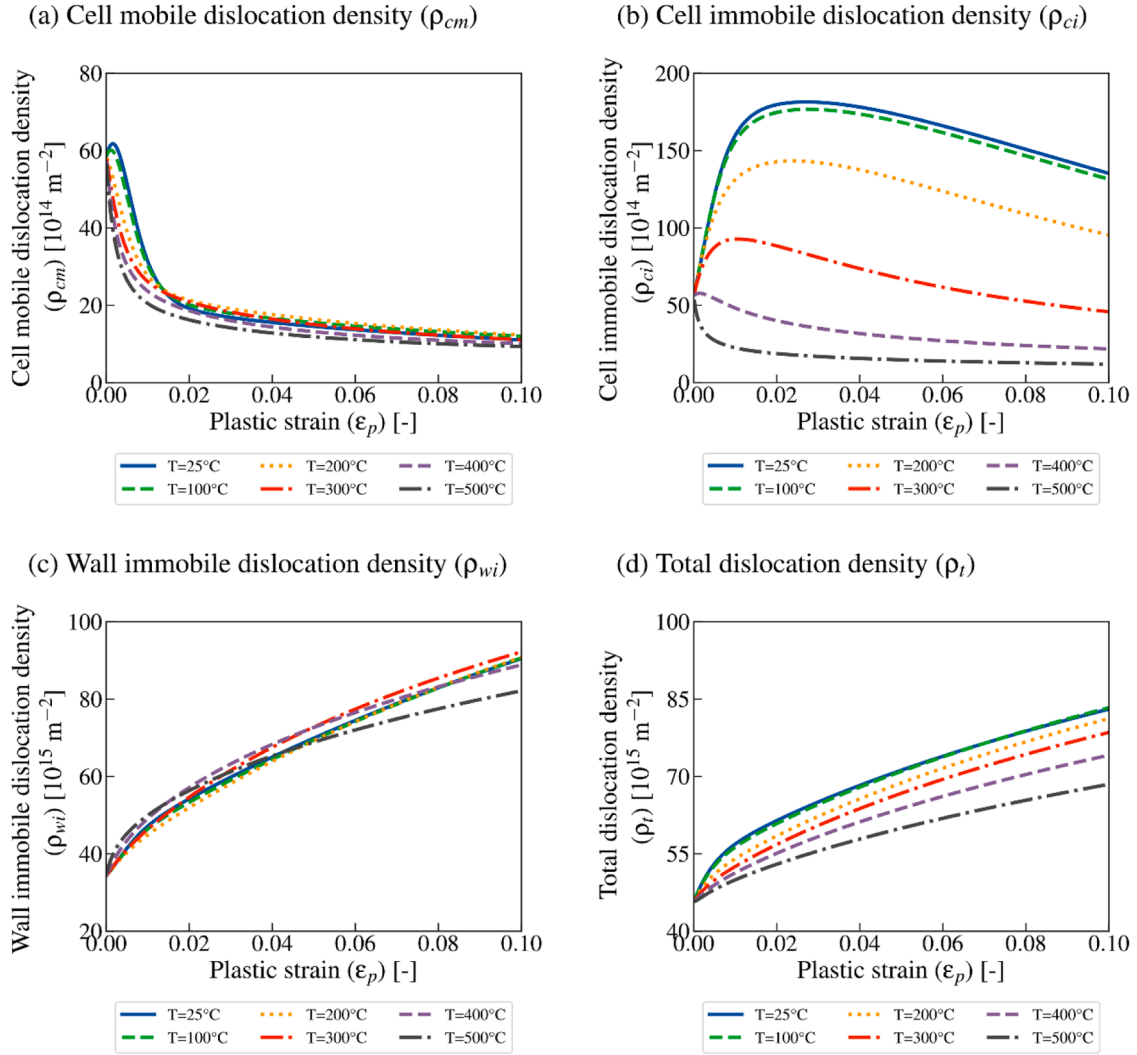


Fig. 12. Evolution of dislocation densities: (a) cell mobile, (b) cell immobile, (c) wall immobile and (d) total dislocations at various temperatures and reference strain rate.

5.5.1. Temperature-Dependent Correction Matrix

To accurately model the behavior of GTN parameters under varying thermal conditions, a temperature-dependent correction matrix is formulated. This matrix combines material-specific constants with temperature-dependent coefficients, providing a systematic approach to compute corrected values for each parameter. The correction accounts for different temperature regimes ($T \leq 300^\circ\text{C}$ and $T > 300^\circ\text{C}$).

Parameter Matrix and Correction Factors

The parameter matrix, P , encapsulates the material-specific constants and the temperature variable T_n . The temperature-dependent correction factors are computed by multiplying the appropriate coefficient matrix (C_{low} or C_{high}) with the parameter matrix P :

$$C(T_n).P; P = \begin{bmatrix} f_c \\ f_f \\ f_N \\ s_n \\ \varepsilon_N \\ T_n \end{bmatrix}, \quad (92)$$

Coefficient Matrices

Two coefficient matrices are defined to capture the linear and non-linear dependencies on temperature for two distinct regimes:

$$\text{For } T \leq 300^\circ\text{C } C_{low} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0.00007 \\ 0 & 1 & 0 & 0 & 0 & 0.0005 \\ 0 & 0 & 1.1 & 0 & 0 & 0.0001 \\ 0 & 0 & 0 & 1 & 0 & -0.0001 \\ 0 & 0 & 0 & 0 & 1.3 & -0.00022 \end{bmatrix}, \quad (93)$$

$$\text{For } T > 300^\circ\text{C } C_{high} = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0.00036 \\ 0 & 1 & 0 & 0 & 0 & 0.0005 \\ 0 & 0 & 0.2 & 0 & 0 & -0.00001 \\ 0 & 0 & 0 & 4 & 0 & 0.00015 \\ 0 & 0 & 0 & 0 & 1.5 & 0.00022 \end{bmatrix}.$$

5.5.2. Discussions on the sensitivity of damage parameters of S700 steel

In Fig. 14, the results from CoP study evaluates the sensitivity and influence of each input parameter on the final output, providing insights into which factors most significantly impact the model's predictive capability. In this context, a higher CoP value reflects a greater contribution of the parameter to the overall variability of the model's output. The results indicate that the void nucleation volume fraction f_N has the highest CoP value at 34.95%, suggesting it is the most influential parameter in predicting the material's ductile fracture behavior. This

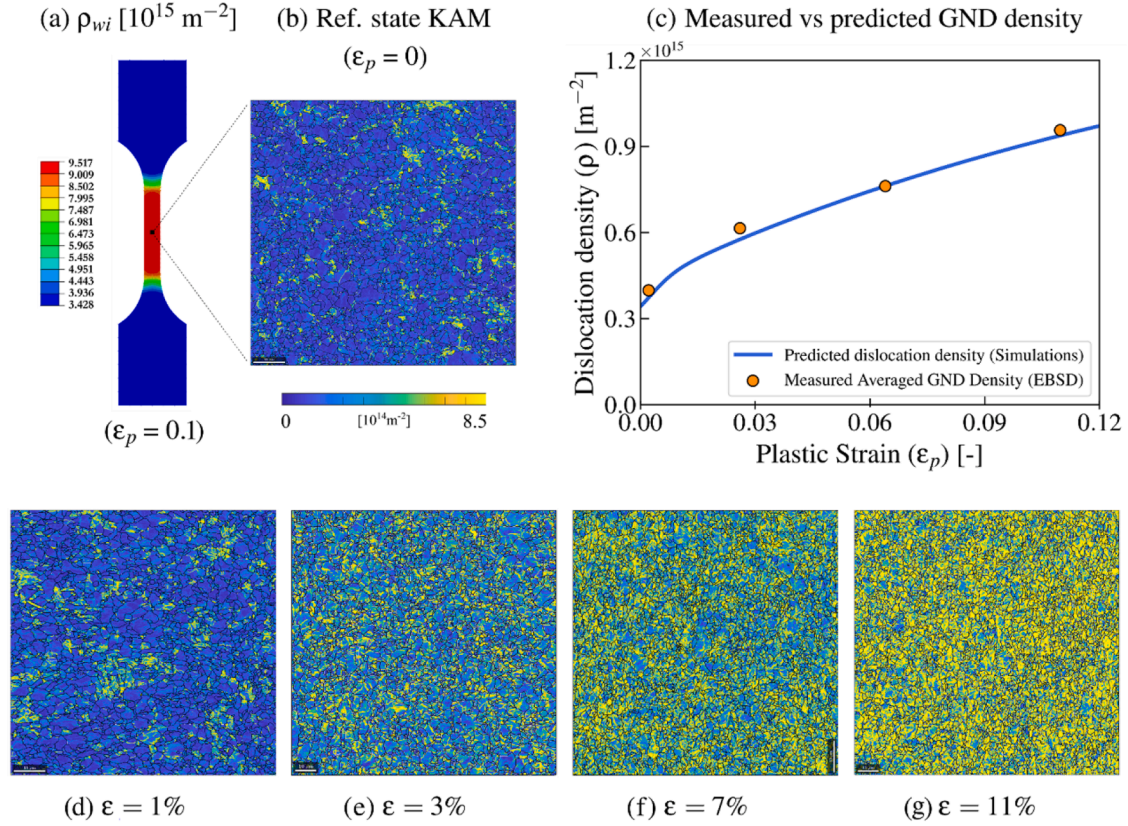


Fig. 13. Comparison between the predicted dislocation density from the RMV based material model and measured GND density from the EBSD measurements.

Table 8
GTN damage parameters.

f_0	f_N	f_c	f_f	q_1	q_2	q_3	s_N	ϵ_N
0.00082	0.02872	0.05564	0.24025	1.66706	0.97297	2.779089	0.07575	0.1815

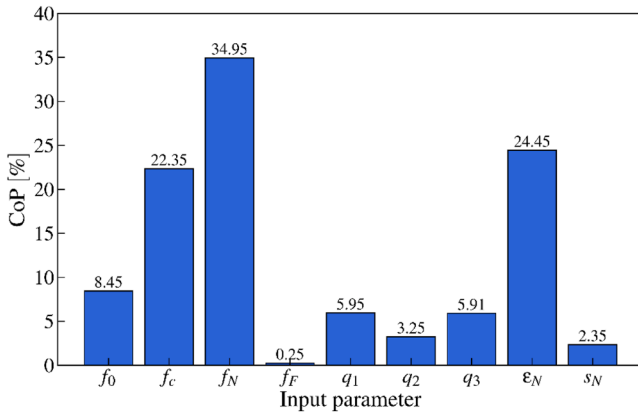


Fig. 14. The coefficient of prognosis (CoP) values for each input parameter of the GTN damage model.

parameter directly impacts the number of voids that form as the material deforms. A higher f_N value implies a greater propensity for voids to nucleate, which can significantly affect the initiation of ductile fracture. The void nucleation strain ϵ_N , with a CoP value of 24.45%, also plays a critical role. This parameter determines the strain at which voids begin to nucleate within the material. A lower ϵ_N means that voids will start forming at lower strains, potentially leading to earlier onset of damage

and eventual fracture.

The critical void volume fraction f_c , with a CoP value of 22.35%, is another important parameter. This parameter represents the void volume fraction at which the material transitions from void growth to void coalescence, a critical phase where individual voids link up, leading to the formation of macroscopic cracks. The higher the f_c , the more void growth is needed before coalescence, which can delay the onset of catastrophic failure. On the other hand, the void volume fraction at final fracture f_f has a negligible CoP value of 0.25%, indicating minimal impact on the model's predictive capability. This suggests that the exact void volume fraction at final fracture is less critical for predicting overall behaviour compared to other parameters like f_N and f_c .

The initial void volume fraction f_0 has a CoP value of 8.45%, indicating its moderate importance. This parameter represents the pre-existing voids in the material before deformation starts. While it influences the initial stage of void growth, its impact is less pronounced than the nucleation and coalescence parameters. The material constants q_1 , q_2 , and q_3 are included to account for the stress state and its effect on void growth. q_1 and q_3 have moderate influence with CoP values of 5.95% and 5.91%, respectively, indicating their role in accurately modelling the influence of hydrostatic stress and the matrix material's hardening behaviour on void growth. q_2 has a lower CoP value of 3.25%, suggesting that variations in this parameter have a lesser effect on the model's accuracy. Finally, the standard deviation of the void nucleation strain s_N has a low CoP value of 2.35%, indicating that variability in the nucleation strain has a minor effect on the overall damage prediction.

In conclusion, the analysis highlights that the parameters governing void nucleation and coalescence play a pivotal role in the model's sensitivity and predictive accuracy, with the void nucleation volume fraction f_N emerging as the most influential factor. This finding underscores that the damage mechanism in S700 steel is primarily dominated by void nucleation, which significantly impacts the initiation and progression of ductile fracture under deformation.

5.5.3. Discussions on the damage mechanisms of S700

This section investigates the damage mechanisms in S700 steel during tensile deformation, with a focus on the necking zone prior to failure. Metallographic analysis of interrupted tensile test samples, extracted specifically from the necking region, provides critical insights into void nucleation, growth, and coalescence, which are the dominant mechanisms underlying ductile damage in high-strength steels.

Ductile failure in high-strength steels, such as S700, is predominantly driven by void nucleation and growth, consistent with previous findings [130–133]. Voids nucleate at various microstructural features, including grain boundaries [134], slip bands, inclusions, and precipitates [135, 136]. However, void nucleation has also been observed in the absence of particles, emphasizing diverse initiation mechanisms. Gardner et al. [137] experimentally demonstrated the significant role of dislocations in void formation, highlighting the importance of dislocation dynamics in the damage evolution of S700 steel.

Fig. 15 presents LOM images of tensile samples interrupted at different strain levels, illustrating the progression of void formation during tensile deformation. At lower strains Fig. 15a, voids are sparse and primarily localized at stress concentrators, such as inclusions or

secondary phases. In the intermediate strains (Fig. 15b-c), void density increases as deformation progresses, with existing voids growing and new voids nucleating. This stage reflects intensified stress concentration and localized deformation around microstructural inhomogeneities and at higher strains (Fig. 15d), void coalescence becomes evident, as neighboring voids interact and merge, marking a transition from growth-dominated to coalescence-driven damage mechanisms. This coalescence signals the onset of macroscopic fracture.

Fig. 16 provides detailed microstructural evidence of the damage mechanisms observed in S700 steel. Stress concentrations at particle-matrix interfaces lead to decohesion, initiating void formation - Hard particles, inclusions, or secondary phases are common nucleation sites, which can be seen in Fig. 16 (a-d). Grain boundaries, particularly in materials with weak cohesion or anisotropic structures, act as stress concentrators, leading to void nucleation via intergranular decohesion (Fig. 16d). Under continued deformation, neighboring voids merge to form larger cavities, accelerating the transition to macroscopic failure (Fig. 16c).

These observations underscore the interplay between microstructural features and tensile stress in driving material degradation. The increasing void volume fraction and subsequent coalescence highlight the critical role of dislocation dynamics, stress redistribution, and microstructural interactions in S700 steel's ductile failure mechanisms.

5.6. Isothermal uniaxial tensile test with damage

The D-TMM model enables a detailed visualization of both macroscopic and microstructural distributions under tensile loading,

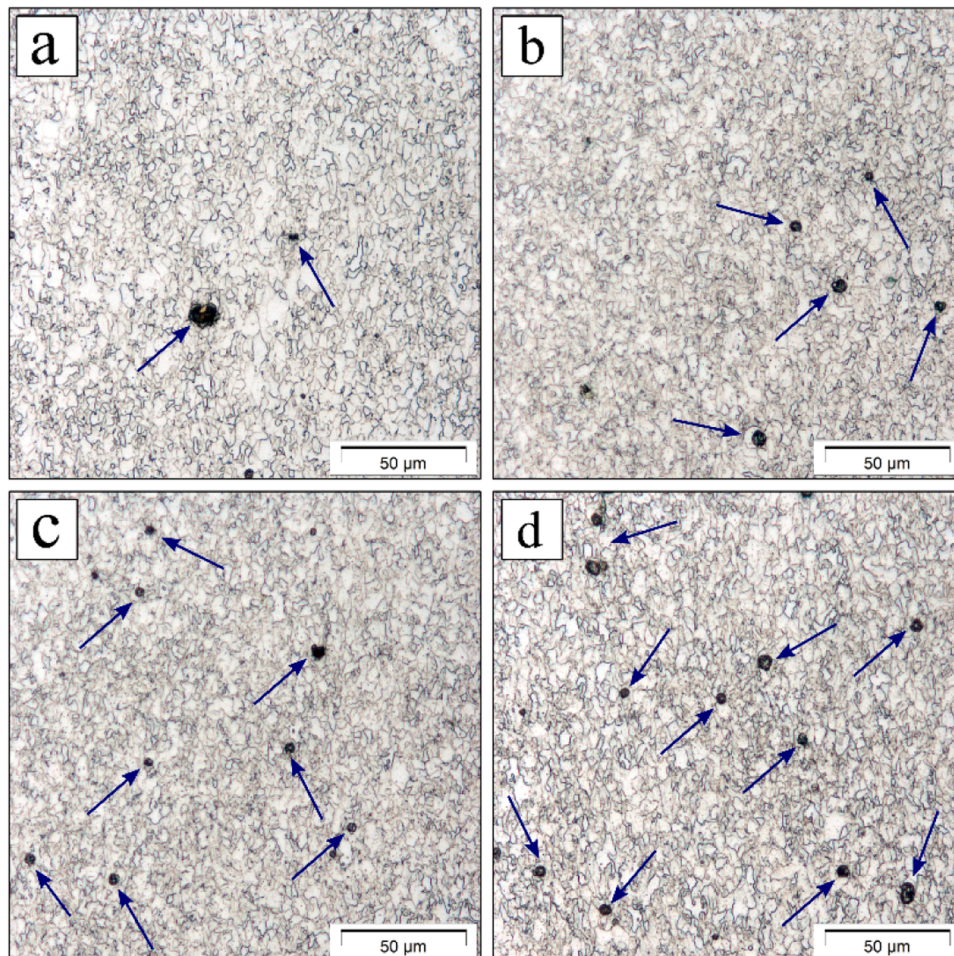


Fig. 15. LOM images of void distribution in the tensile samples interrupted at various strains: (a) 15%, (b) 17%, (c) 19%, and (d) 21%.

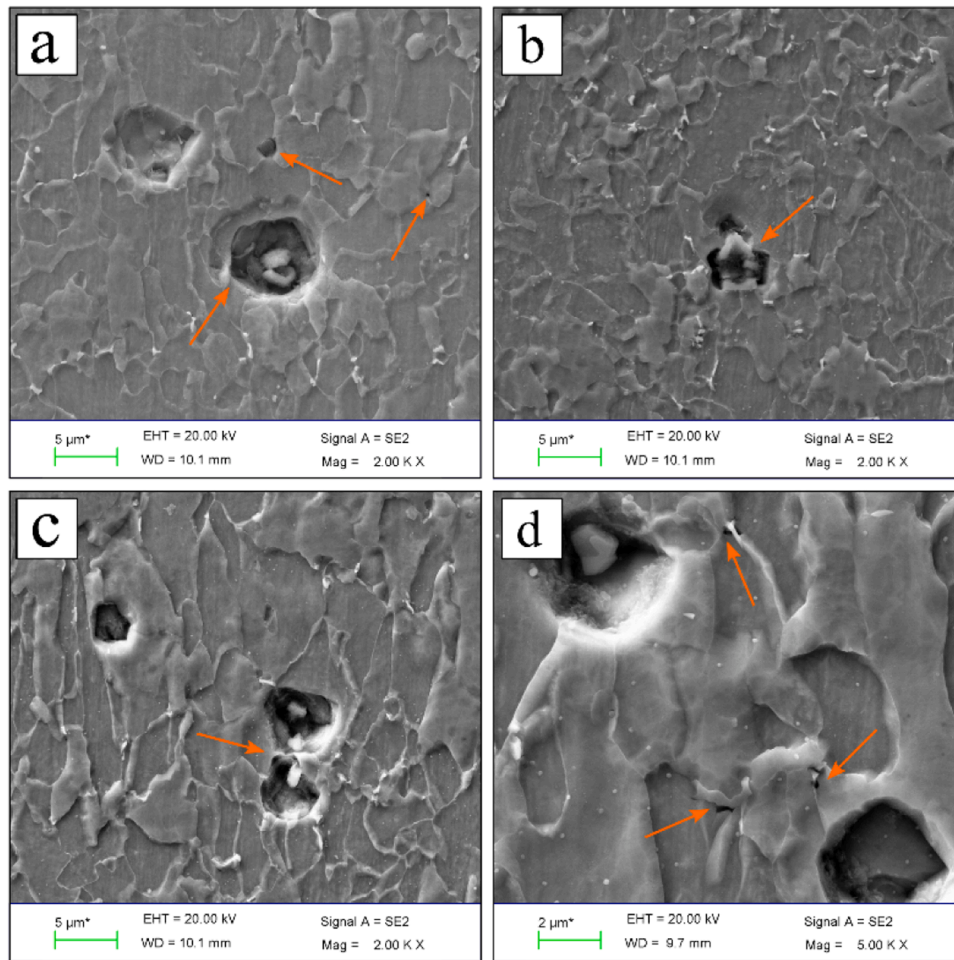


Fig. 16. Voids formed during the ductile damage process through different mechanisms: (a) voids nucleating and growing at the site of a particle, (b) a particle nucleating a void, (c) two voids coalescing to propagate damage, and (d) void formation at grain boundaries due to decohesion.

providing essential correlations for understanding material behaviour across scales. FE simulations, conducted at reference temperature and strain rate, capture the tensile response of S700 steel at a critical point where damage initiation and propagation have begun, as shown in Fig. 17.

The equivalent plastic strain field (Fig. 17e) reveals regions of significant strain localization, concentrated around the necking zone, indicating fracture. This distribution highlights the material's capacity for plastic deformation before failure, with high plastic strain regions aligning with typical crack nucleation sites. By examining these strain localizations, we can identify areas most susceptible to damage initiation, confirming the accumulation of irreversible deformation leading up to crack onset.

The stress field (Fig. 17a), represented by $\bar{\sigma}$, shows localized stress concentrations also around the necking zone, where peak stress reaches approximately 1058 MPa. This stress localization corresponds with expected crack initiation sites, underscoring the importance of stress-driven mechanisms in the failure process. The void volume fraction f distribution (Fig. 17f) provides further insights into microstructural changes, showing high void densities near the specimen centre, where strain and stress concentrate, facilitating void coalescence and crack formation. This progression of void growth and coalescence characterizes ductile fracture, with the D-TMM model accurately representing the impact of micro voids in driving damage accumulation.

In terms of dislocation behaviour, the distribution of cell mobile, cell immobile, and wall immobile dislocations (Fig. 17 (b-d)) across the deformation zone offers insights into dislocation dynamics at the ductile

damage site. Within the necking zone, high equivalent stress and plastic strain localizations lead to a depletion of cell mobile and cell immobile dislocations and an accumulation of wall immobile dislocations. As the material undergoes plastic deformation, dynamic annihilation reduces cell mobile dislocation density. While cell immobile dislocation density initially peaks at lower strains (Fig. 12b), it subsequently decreases in heavily deformed areas, particularly in the necking zone. Observing regions above and below the necking zone highlights this behaviour. During deformation, mobile dislocations that escape annihilation become trapped by interstitial atoms, and in combination with certain cell immobile dislocations, they contribute to wall immobile dislocation nucleation. This accumulation of wall dislocations intensifies localized stress and strain (Fig. 17d), promoting void formation and contributing to the material's ductile fracture behaviour.

Overall, the D-TMM model effectively captures stress heterogeneity and dislocation-driven mechanisms, providing a comprehensive view of the interplay between dislocation evolution, void formation, and ductile damage initiation and propagation.

5.6.1. Discussions on damage progression in tensile loading

Fig. 18 illustrates the isothermal tensile test simulation results for S700 steel, focusing on damage initiation and failure mechanisms. Fig. 18(a) shows a comparison of the engineering stress-strain curve obtained from experimental data and simulated results under identical conditions. The close agreement between the experimental (solid line) and simulated (dotted line) curves validate the accuracy of the D-TMM model in capturing the material's deformation and failure behavior.

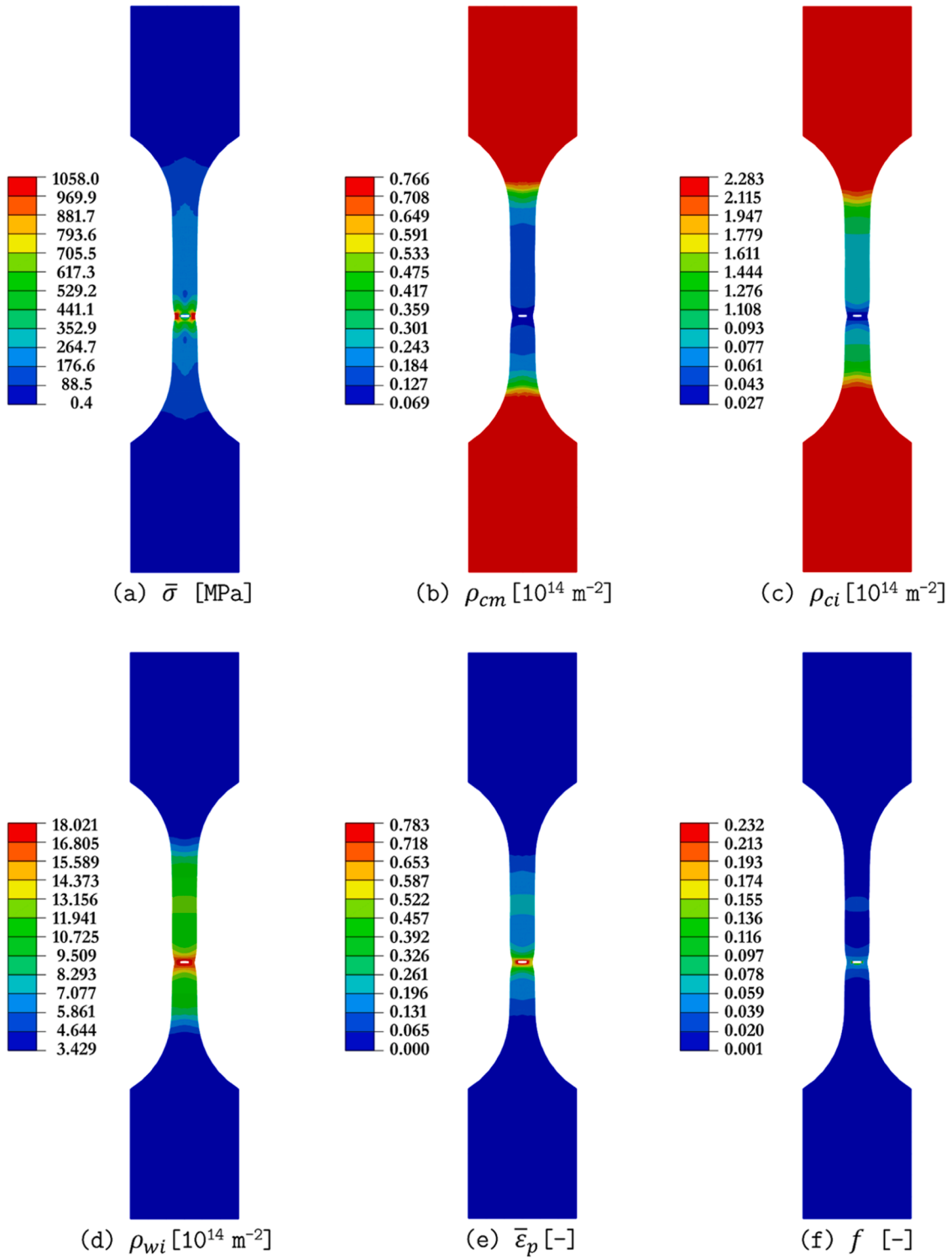


Fig. 17. Results from FE simulation of isothermal tensile test in the damage dominated regime using the D-TMM material model at reference temperature and strain rate.

Fig. 18(b) tracks the evolution of wall immobile dislocation density ρ_{wi} and void fraction f as functions of engineering strain. Wall dislocation density increases steadily with strain, reflecting the progressive accumulation of dislocations during plastic deformation. Meanwhile, the void fraction remains low initially but rises sharply near fracture, signaling the nucleation and growth of voids as precursors to failure.

Fig. 18 (c-e) depicts the spatial distribution of voids at different strain levels ($\epsilon = 22.5\%$, 24.0% , 25.5%). At $\epsilon = 22.5\%$, voids begin to nucleate

in the necking region. As the strain reaches $\epsilon = 24.0\%$, voids grow and start coalescing, leading to material weakening. At $\epsilon = 25.5\%$, extensive void coalescence results in complete fracture, forming a distinct fracture surface. Damage localization is observed below the specimen's center (as seen in Fig. 18), which is due to dynamic effects at a strain rate of 0.1 s^{-1} . In the necking zone, rapid strain rate increases heighten sensitivity, which could delay stress redistribution due to insufficient relaxation time. Both experimental and simulation results confirm failure initiation

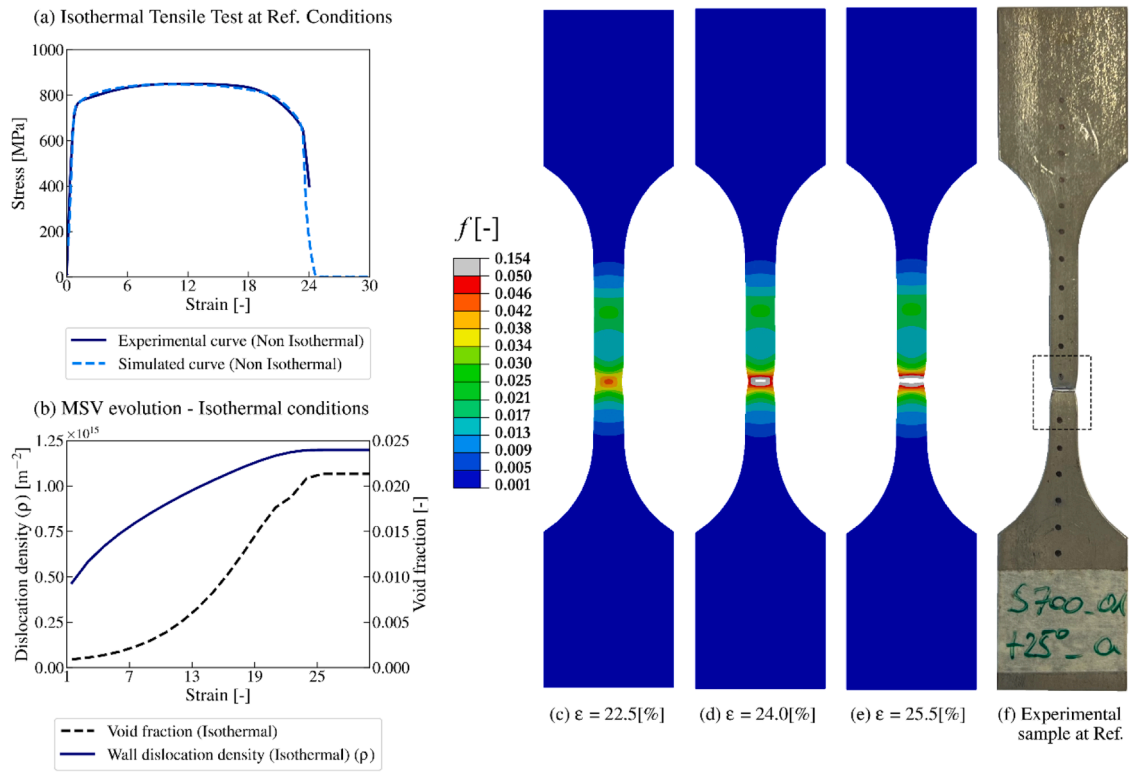


Fig. 18. Results from the isothermal tensile test experiments and simulations: (a) Engineering stress-strain curves obtained from experiments and simulations for reference conditions; (b) MSV evolution during the tensile test; (c-e): Damage localization and progression during the tensile test; (f): Experimental tensile test sample for the same conditions.

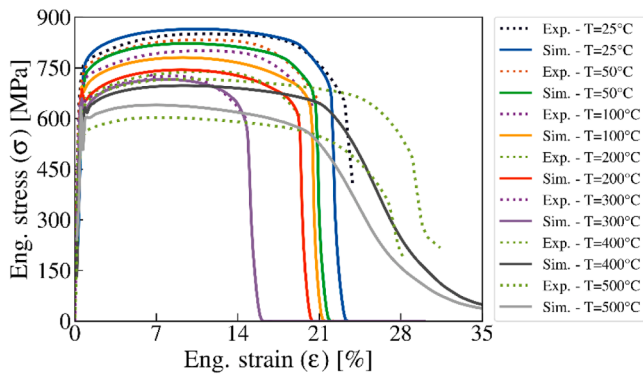


Fig. 19. Engineering stress-strain curves from experimental investigations under isothermal conditions at 25 °C, 50 °C, 100 °C, 200 °C, 300 °C, 400 °C, and 500 °C, accompanied by FE-predicted curves using the D-TMM model for the same conditions.

at this localized region (Fig. 18 (c-f)).

5.7. Thermal effects on GTN damage parameters

In this section, we investigate the predictive capability of the D-TMM model for uniaxial tensile testing across different temperatures. Using the FE model described in Section 5.6, isothermal simulations were conducted for temperatures ranging from 25 °C to 500 °C at the reference strain rate. These simulations offer insights into the underlying dynamics of dislocation evolution and void fraction development, contributing to the material's softening and damage behavior at intermediate and warm temperatures. Experimental uniaxial tensile responses of S700 steel are compared with the model predictions.

In the cold regime (curves: T25 °C, T50 °C, and T100 °C in Fig. 19),

yield stress decreases with temperature, attributed primarily to reductions in viscous stress as a component of dynamic thermal softening (DTS) as described in Section 5.1.1. As temperature increases, dislocation annihilation progresses through cross-slip mechanisms, while wall immobile dislocations accumulate. This accumulation arises as mobile dislocations become trapped or immobilized at barriers such as grain boundaries and pre-existing dislocations, subsequently integrating into cell walls. Increased wall immobile dislocation density promotes work hardening by impeding further dislocation motion, enhancing strength but reducing ductility. High densities of immobile dislocations create localized stress concentrations, which can serve as sites for void nucleation (Section 5.5.2), evidenced by earlier damage initiation at elevated temperatures.

In the intermediate regime (curves: T200 °C and T300 °C in Fig. 19), dynamic thermal hardening (DTH) becomes more influential due to increased dynamic trapping of cell mobile dislocations and intensified wall immobile dislocation nucleation, as shown in Fig. 7(d) and (e). This effect is reflected in the yield points for T200 °C and T300 °C, which converge as DTH strengthens (also can be seen in Fig. 10c). At 300 °C, remobilization of cell immobile dislocations and a surge in wall dislocation nucleation are observed (Fig. 7 (e-g)). This reduces ductility further, as intensified wall immobile dislocation nucleation accelerates damage evolution.

In the warm regime (curves: T400 °C and T500 °C in Fig. 19), the stress-strain curves exhibit notable decreases in peak stress and extended plastic deformation before failure. The decrease in yield stresses at high temperatures corresponds to reduced interaction strengths and diminished viscous stress (Fig. 8). At these temperatures, remobilization of cell immobile and wall immobile dislocations intensifies (Fig. 7f and g); however, the impact of wall dislocation nucleation is comparatively minimal due to the predominance of remobilized dislocations. Consequently, the influence of dislocation density on void nucleation diminishes, leading to enhanced softening before failure. The extent of cell

mobile dislocation annihilation also increases significantly (Fig. 7a), facilitating greater dislocation motion and plastic deformation, which drives void growth. This behavior is reflected in the stress-strain curves gradual decline, indicating that void growth and coalescence dominate failure mechanisms at high temperatures.

The D-TMM model effectively predicts the stress-strain response of S700 steel across low to moderate temperatures (25 °C to 300 °C), accurately capturing yield stress, work hardening, and damage evolution. At lower temperatures, the model replicates high dislocation density and void nucleation, while at intermediate temperatures, it balances dislocation dynamics with void growth. However, at higher temperatures (400 °C to 500 °C), model predictions slightly deviate, reflecting limitations in simulating extensive material softening and plastic deformation. These discrepancies suggest the need for incorporating dynamic recrystallization and advanced void growth mechanisms to enhance predictive accuracy.

5.8. Non-Isothermal uniaxial tensile tests with damage

The aim of simulating non-isothermal tests using the developed D-TMM model in FE simulations is to test and validate the model's predictive capability, as real-world processes often involve heating due to deformation, which affects the material behavior. Non-isothermal tensile tests were conducted on the same standard sample used for isothermal tensile tests (Section 4.2), with which the model parameters were validated. For these simulations, the FE simulation model of uniaxial tensile test as described in Section 5.2 was utilized along with the VUMAT subroutine to incorporate the D-TMM material model. The mechanical and physical properties of the material, i.e., elastic modulus, Poisson's ratio, mass density, specific heat capacity, thermal conductivity, and thermal expansion, were inputted into the FE model as functions of temperature. Additionally, appropriate convection and radiation mechanisms were defined to accurately simulate the thermal environment.

Non-uniform temperature distribution during the tensile test can create thermal stress concentrations, which can act as nucleation sites for voids. These stress concentrations enhance the local plastic deformation, further accelerating void nucleation and growth. At elevated temperatures, the amplitude of wall immobile dislocation nucleation increases (Fig. 7e), promoting the nucleation of voids. Increased annihilation and remobilization of cell immobile dislocations (Fig. 7b and f),

results in increased mobile dislocations, thus allowing voids to grow faster and coalesce at lower strain levels compared to the isothermal case. The combined effects of increased dislocation mobility, thermal softening, and void nucleation contribute to the earlier onset of damage in the non-isothermal case, leading to premature failure (Fig. 20).

6. Conclusions

This study presents a comprehensive framework for analysing deformation and damage mechanisms in S700 steel by integrating a dislocation density-based thermo-micro-mechanical (TMM) model [1] with the Gurson-Tvergaard-Needleman (GTN) damage framework. The approach captures the material's behaviour under tensile deformation across various temperatures and strain rates, combining dislocation dynamics and void fraction evolution to provide a multiscale perspective linking microstructural mechanisms to macroscopic responses.

The D-TMM model effectively tracks the evolution of microstructural state variables, such as cell mobile, cell immobile, wall immobile dislocation densities and void fraction, and correlates these with stress-strain behaviour. Validation of dislocation density predictions through EBSD measurements confirms the model's capability to accurately describe microstructural changes up to the damage initiation threshold. Isothermal tensile test simulations reveal the interplay between dynamic thermal softening (DTS) and dynamic thermal hardening (DTH), influencing yield stress, hardening capacity, and ductility across varying temperature regimes.

GTN model parameters, calibrated through sensitivity analyses and validated against experimental force curves, enhance the framework's ability to predict damage initiation and progression. Coefficient of Prognosis (CoP) analysis identifies void nucleation f_N as a critical factor governing ductile fracture, highlighting the pivotal role of micro void dynamics in the material's failure mechanisms. Metallographic analyses of interrupted tensile tests further validate the model, demonstrating void nucleation, growth, and coalescence as primary drivers of ductile damage. The observed transition from stress concentration-induced void nucleation to void interaction and coalescence aligns well with the model's predictions, showcasing its robustness.

Temperature-dependent mechanisms are well-captured, with DTS effects reducing yield stress and ductility at lower temperatures, DTH mechanisms increasing strength but reducing ductility at intermediate temperatures, and intensified remobilization and annihilation causing

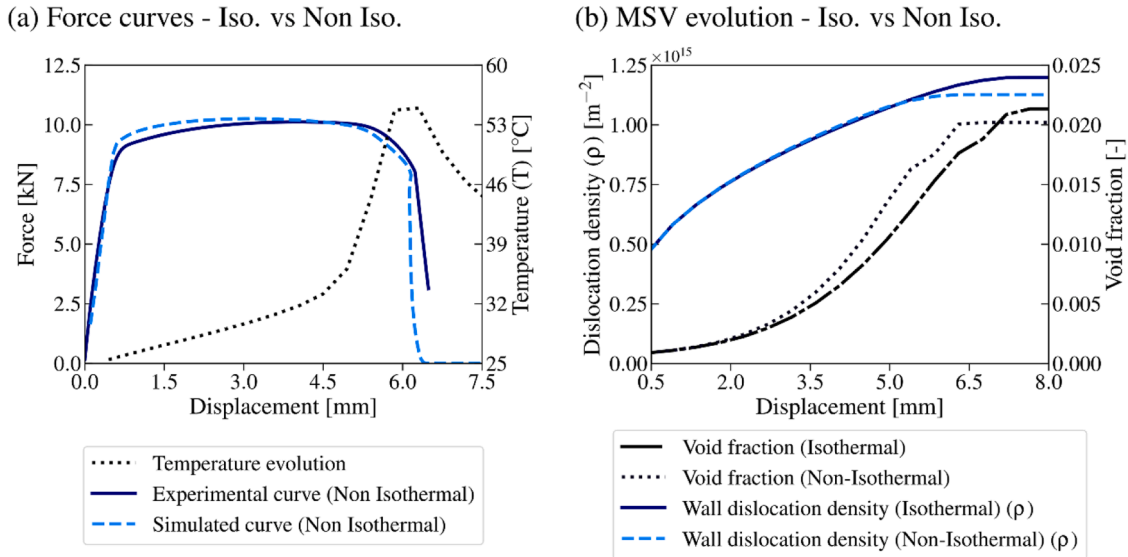


Fig. 20. Non-isothermal uniaxial tensile tests conducted under reference conditions include: (a) force-displacement curves from experimental investigations and FE predictions, accompanied by temperature evolution; (b) comparison of the evolution of dislocation density between two cases – Isothermal and Non Isothermal conditions.

softening and extensive plastic deformation at warm temperatures. However, the model's limitations become apparent at higher temperatures, where it struggles to address dynamic recrystallization and advanced void growth processes. Incorporating mechanisms like grain boundary migration and enhanced void interactions could extend its predictive accuracy in these regimes.

In conclusion, the integrated D-TMM framework offers a robust approach for understanding the deformation and damage behaviour of S700 steel. By capturing the coupling between microstructural evolution and macroscopic responses, the model provides valuable insights for optimizing the performance of high-strength steels in demanding applications. Furthermore, it lays the groundwork for extending multiscale modelling approaches to other material systems and complex loading scenarios, advancing the predictive capability of ductile damage mechanisms.

CRedit authorship contribution statement

Karthik Ramalingam: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **S. Amir H. Motaman:** Conceptualization. **Christian Haase:** Writing – review & editing, Supervision,

Methodology. **Ulrich Krupp:** Writing – review & editing, Supervision, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported on this paper.

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Appendix 1

The derivatives mentioned in Section 3.4 is solved as follows:

$$J_{11} = \frac{\partial R_1}{\partial \Delta \bar{\epsilon}_p} = \theta \left[4q_1 f^* \sigma_y \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) - 2\sigma_y (1 + q_3 f^{*2}) - 3q_1^2 f^* \sigma_h \sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \right] = 0 \quad (\text{A.1})$$

$$J_{12} = \frac{\partial R_1}{\partial \Delta \lambda} = \frac{-12G\bar{\sigma}_r^2}{(1 - 6G\Delta\lambda)^3} \quad (\text{A.2})$$

$$J_{13} = \frac{\partial R_1}{\partial \sigma_h} = 3q_1 q_2 f^* \sigma_y \sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \quad (\text{A.3})$$

$$J_{14} = \frac{\partial R_1}{\partial f} = 2\sigma_y^2 \left[q_1 \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) - q_3 f^{*2} \right] \frac{\partial f^*}{\partial f} \quad (\text{A.4})$$

$$J_{15} = \frac{\partial R_1}{\partial \hat{\rho}_{cm}} = 0; \quad J_{16} = \frac{\partial R_1}{\partial \hat{\rho}_{ci}} = \frac{\sigma_{pc}}{2\hat{\rho}_{ci}}; \quad J_{17} = \frac{\partial R_1}{\partial \hat{\rho}_{cm}} = \frac{\sigma_{pw}}{2\hat{\rho}_{wi}} \quad (\text{A.5})$$

$$J_{21} = \frac{\partial R_2}{\partial \Delta \bar{\epsilon}_p} = 3q_1 q_2 (1 - f) f^* \Delta \lambda \theta \left(\sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) - \frac{3q_2 \sigma_h}{2\sigma_y} \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \right) + A = 0 \quad (\text{A.6})$$

$$J_{22} = \frac{\partial R_2}{\partial \Delta \lambda} = 3q_1 q_2 (1 - f) f^* \sigma_y \sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \quad (\text{A.7})$$

$$J_{23} = \frac{\partial R_2}{\partial \sigma_h} = \frac{9}{2} q_1 q_2^2 (1 - f) f^* \Delta \lambda \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) + \Delta \bar{\epsilon}_p \frac{\partial A}{\partial \sigma_h} \quad (\text{A.8})$$

$$J_{24} = \frac{\partial R_2}{\partial f} = 3q_1 q_2 \sigma_y \Delta \lambda \sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \left[(1 - f) \frac{\partial f^*}{\partial f} - f^* \right] - 1 \quad (\text{A.9})$$

$$J_{25} = \frac{\partial R_2}{\partial \hat{\rho}_{cm}} = 0 \quad (\text{A.10})$$

$$J_{26} = \frac{\partial R_2}{\partial \hat{\rho}_{ci}} = 3q_1 q_2 (1 - f) f^* \Delta \lambda \left(\sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) - \frac{3q_2 \sigma_h}{2\sigma_y} \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \right) \frac{\sigma_{pc}}{2\hat{\rho}_{ci}} \quad (\text{A.11})$$

$$J_{27} = \frac{\partial R_2}{\partial \hat{\rho}_{cm}} = 3q_1 q_2 (1 - f) f^* \Delta \lambda \left(\sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) - \frac{3q_2 \sigma_h}{2\sigma_y} \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \right) \frac{\sigma_{pw}}{2\hat{\rho}_{wi}} \quad (\text{A.12})$$

$$J_{31} = \frac{\partial R_3}{\partial \Delta \bar{\epsilon}_p} = 3q_1 q_2 f^* \sigma_h \Delta \lambda \theta \left(\sinh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) - \frac{3q_2 \sigma_h}{2\sigma_y} \cosh\left(\frac{3q_2 \sigma_h}{2\sigma_y}\right) \right) - (1 - f) (\sigma_y + \theta \Delta \bar{\epsilon}_p) = 0 \quad (\text{A.13})$$

$$J_{32} = \frac{\partial R_3}{\partial \Delta \lambda} = \frac{2\bar{\sigma}_r^2(1 - 6G\Delta\lambda)}{(1 + 6G\Delta\lambda)^3} + 3q_1q_2f^*\sigma_y\sigma_h\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) \quad (\text{A. 14})$$

$$J_{33} = \frac{\partial R_3}{\partial \sigma_h} = 3q_1q_2f^*\sigma_y\Delta\lambda\left(\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) + \frac{3q_2\sigma_h}{2\sigma_y}\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\right) \quad (\text{A. 15})$$

$$J_{34} = \frac{\partial R_3}{\partial f} = 3q_1q_2\sigma_y\sigma_h\Delta\lambda\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\frac{\partial f^*}{\partial f} + \sigma_y\Delta\bar{\epsilon}_p \quad (\text{A. 16})$$

$$J_{35} = \frac{\partial R_3}{\partial \hat{\rho}_{cm}} = 0 \quad (\text{A. 17})$$

$$J_{36} = \frac{\partial R_3}{\partial \hat{\rho}_{ci}} = 3q_1q_2f^*\sigma_h\Delta\lambda\left(\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) - \frac{3q_2\sigma_h}{2\sigma_y}\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\right)\frac{\sigma_{pc}}{2\hat{\rho}_{ci}} - (1-f)\Delta\bar{\epsilon}_p\frac{\sigma_{pc}}{2\hat{\rho}_{ci}} \quad (\text{A. 18})$$

$$J_{37} = \frac{\partial R_3}{\partial \hat{\rho}_{cm}} = 3q_1q_2f^*\sigma_h\Delta\lambda\left(\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) - \frac{3q_2\sigma_h}{2\sigma_y}\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\right)\frac{\sigma_{pw}}{2\hat{\rho}_{wi}} - (1-f)\Delta\bar{\epsilon}_p\frac{\sigma_{pw}}{2\hat{\rho}_{wi}} \quad (\text{A. 19})$$

$$J_{41} = \frac{\partial R_4}{\partial \Delta\bar{\epsilon}_p} = 3q_1q_2f^*K\Delta\lambda\theta\left(\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) - \frac{3q_2\sigma_h}{2\sigma_y}\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\right) = 0 \quad (\text{A. 20})$$

$$J_{42} = \frac{\partial R_4}{\partial \Delta\lambda} = 3q_1q_2f^*\sigma_yK\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) \quad (\text{A. 21})$$

$$J_{43} = \frac{\partial R_4}{\partial \sigma_h} = 1 + \frac{9}{2}q_1q_2^2f^*K\Delta\lambda\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) \quad (\text{A. 22})$$

$$J_{44} = \frac{\partial R_4}{\partial f} = 3q_1q_2\sigma_yK\Delta\lambda\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\frac{\partial f^*}{\partial f} \quad (\text{A. 23})$$

$$J_{45} = \frac{\partial R_4}{\partial \hat{\rho}_{cm}} = 0 \quad (\text{A. 24})$$

$$J_{46} = \frac{\partial R_4}{\partial \hat{\rho}_{ci}} = 3q_1q_2f^*K\Delta\lambda\theta\left(\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) - \frac{3q_2\sigma_h}{2\sigma_y}\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\right)\frac{\sigma_{pc}}{2\hat{\rho}_{ci}} \quad (\text{A. 25})$$

$$J_{47} = \frac{\partial R_4}{\partial \hat{\rho}_{cm}} = 3q_1q_2f^*K\Delta\lambda\theta\left(\sinh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right) - \frac{3q_2\sigma_h}{2\sigma_y}\cosh\left(\frac{3q_2\sigma_h}{2\sigma_y}\right)\right)\frac{\sigma_{pw}}{2\hat{\rho}_{wi}} \quad (\text{A. 26})$$

$$J_{51} = \frac{\partial R_5}{\partial \Delta\bar{\epsilon}_p} = -\Delta\hat{\rho}_{cm} - m_{ci}^{rm}\Delta\hat{\rho}_{ci}^{rm} - m_{wi}^{rm}\Delta\hat{\rho}_{wi}^{rm} + 2m_{cm}^{an}\Delta\hat{\rho}_{an}^{cm} + m_{ci}^{an}\Delta\hat{\rho}_{ci}^{an} + m_{wi}^{an}\Delta\hat{\rho}_{wi}^{an} + m_{cm}^{tr}\Delta\hat{\rho}_{cm}^{tr} \quad (\text{A. 27})$$

$$J_{52} = \frac{\partial R_5}{\partial \Delta\lambda} = 0; J_{53} = \frac{\partial R_5}{\partial \sigma_h} = 0; J_{54} = \frac{\partial R_5}{\partial f} = 0 \quad (\text{A. 28})$$

$$J_{55} = \frac{\partial R_5}{\partial \hat{\rho}_{cm}} = 1 - \frac{\Delta\bar{\epsilon}_p}{\hat{\rho}_{cm}}\left(\Delta\hat{\rho}_{cm}^{gn} - \left(4\Delta\hat{\rho}_{cm}^{an} + \Delta\hat{\rho}_{ci}^{an} + \Delta\hat{\rho}_{wi}^{an} + \Delta\hat{\rho}_{ci}^{ac} + \Delta\hat{\rho}_{wi}^{ac} + \frac{3}{2}\Delta\hat{\rho}_{cm}^{tr}\right)\right) \quad (\text{A. 29})$$

$$J_{56} = \frac{\partial R_5}{\partial \hat{\rho}_{ci}} = -\frac{\Delta\bar{\epsilon}_p}{\hat{\rho}_{ci}}\left[-\frac{1}{2}\frac{\Delta\hat{\rho}_{cm}^{gn}}{\left(1 + \frac{\hat{\rho}_{wi}}{\hat{\rho}_{ci}}\right)} + \Delta\hat{\rho}_{ci}^{rm} - \left(\Delta\hat{\rho}_{ci}^{an} + \frac{1}{2}\Delta\hat{\rho}_{ci}^{ac}\right)\right] \quad (\text{A. 30})$$

$$J_{57} = \frac{\partial R_5}{\partial \hat{\rho}_{cm}} = -\frac{\Delta\bar{\epsilon}_p}{\hat{\rho}_{wi}}\left[-\frac{1}{2}\frac{\Delta\hat{\rho}_{cm}^{gn}}{\left(1 + \frac{\hat{\rho}_{wi}}{\hat{\rho}_{ci}}\right)} + \Delta\hat{\rho}_{wi}^{rm} - \left(\Delta\hat{\rho}_{wi}^{an} + \frac{1}{2}\Delta\hat{\rho}_{wi}^{ac}\right)\right] \quad (\text{A. 31})$$

$$J_{61} = \frac{\partial R_6}{\partial \Delta\bar{\epsilon}_p} = -\Delta\hat{\rho}_{ci} - m_{cm}^{tr}\Delta\hat{\rho}_{cm}^{tr} + m_{ci}^{an}\Delta\hat{\rho}_{ci}^{an} + m_{wi}^{nc}\Delta\hat{\rho}_{wi}^{nc} + m_{ci}^{rm}\Delta\hat{\rho}_{ci}^{rm} \quad (\text{A. 32})$$

$$J_{62} = \frac{\partial R_6}{\partial \Delta\lambda} = 0; J_{63} = \frac{\partial R_6}{\partial \sigma_h} = 0; J_{64} = \frac{\partial R_6}{\partial f} = 0 \quad (\text{A. 33})$$

$$J_{65} = \frac{\partial R_6}{\partial \hat{\rho}_{cm}} = -\frac{\Delta\bar{\epsilon}_p}{\hat{\rho}_{cm}}\left[\Delta\hat{\rho}_{ci}^{ac} + \frac{3}{2}\Delta\hat{\rho}_{cm}^{tr} - \Delta\hat{\rho}_{ci}^{an} - \Delta\hat{\rho}_{wi}^{nc}\right] \quad (\text{A. 34})$$

$$J_{66} = \frac{\partial R_6}{\partial \hat{\rho}_{ci}} = 1 - \frac{\Delta\bar{\epsilon}_p}{\hat{\rho}_{ci}}\left[\frac{1}{2}\Delta\hat{\rho}_{ci}^{ac} - \Delta\hat{\rho}_{ci}^{an} - \frac{3}{2}\Delta\hat{\rho}_{wi}^{nc} - \Delta\hat{\rho}_{ci}^{rm}\right] \quad (\text{A. 35})$$

$$J_{67} = \frac{\partial R_6}{\partial \hat{\rho}_{cm}} = 0 \quad (\text{A. 36})$$

$$J_{71} = \frac{\partial R_7}{\partial \Delta \bar{\epsilon}_p} = -\Delta \hat{\rho}_{wi} + m_{wi}^{an} \Delta \hat{\rho}_{wi}^{an} - m_{wi}^{nc} \Delta \hat{\rho}_{wi}^{nc} + m_{wi}^{rm} \Delta \hat{\rho}_{wi}^{rm} \quad (\text{A. 37})$$

$$J_{72} = \frac{\partial R_7}{\partial \Delta \lambda} = 0; J_{73} = \frac{\partial R_7}{\partial \sigma_h} = 0; J_{74} = \frac{\partial R_7}{\partial f} = 0 \quad (\text{A. 38})$$

$$J_{75} = \frac{\partial R_7}{\partial \hat{\rho}_{cm}} = -\frac{\Delta \bar{\epsilon}_p}{\hat{\rho}_{cm}} [\Delta \hat{\rho}_{wi}^{ac} - \Delta \hat{\rho}_{wi}^{an} + \Delta \hat{\rho}_{wi}^{nc}] \quad (\text{A. 39})$$

$$J_{76} = \frac{\partial R_7}{\partial \hat{\rho}_{ci}} = -\frac{\Delta \bar{\epsilon}_p}{\hat{\rho}_{ci}} \left[\frac{3}{2} \Delta \hat{\rho}_{wi}^{nc} \right] \quad (\text{A. 40})$$

$$J_{77} = \frac{\partial R_7}{\partial \hat{\rho}_{cm}} = 1 - \frac{\Delta \bar{\epsilon}_p}{\hat{\rho}_{wi}} \left[\frac{1}{2} \Delta \hat{\rho}_{wi}^{ac} - \Delta \hat{\rho}_{wi}^{an} - \Delta \hat{\rho}_{wi}^{rm} \right] \quad (\text{A. 41})$$

Where θ is viscoplastic tangent modulus and it can be calculated as follows,

$$\theta = \frac{\partial \sigma}{\partial \Delta \bar{\epsilon}_p} = \theta_v + \theta_p \quad (\text{A. 42})$$

$$\theta = \frac{\partial \sigma}{\partial \Delta \bar{\epsilon}_p} = \frac{\partial \sigma_v}{\partial \Delta \bar{\epsilon}_p} + \frac{\partial \sigma_p}{\partial \Delta \bar{\epsilon}_p} \quad (\text{A. 43})$$

$$\theta = \frac{\partial \sigma}{\partial \Delta \bar{\epsilon}_p} = \frac{\sigma_v m_v}{\Delta \bar{\epsilon}_p} + \left[\Delta \hat{\rho}_{ci} + (m_{cm}^r \Delta \hat{\rho}_{cm}^r) - (m_{ci}^{an} \Delta \hat{\rho}_{ci}^{an}) - (m_{ci}^{rm} \Delta \hat{\rho}_{ci}^{rm}) - (m_{wi}^{nc} \Delta \hat{\rho}_{wi}^{nc}) \right] \frac{\sigma_{pc}}{2 \hat{\rho}_{ci}} + \left[\Delta \hat{\rho}_{wi} + (m_{wi}^{nc} \Delta \hat{\rho}_{wi}^{nc}) - (m_{wi}^{an} \Delta \hat{\rho}_{wi}^{an}) - (m_{wi}^{rm} \Delta \hat{\rho}_{wi}^{rm}) \right] \frac{\sigma_{pw}}{2 \hat{\rho}_{wi}} \quad (\text{A. 44})$$

Data availability

Data will be made available on request.

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