

On the grain level deformation of BCC metals with crystal plasticity modeling: Application to an RPV steel and the effect of irradiation

Matti Lindroos^{a,*}, Guilherme Corrêa Soares^a, Abhishek Biswas^a, Wade Karlsen^a,
Andris Freimanis^a, Sicong Ren^a, Marta Serrano^b, Anssi Laukkanen^a

^a VTT Technical Research Centre Of Finland Ltd., Tekniikantie 21, Espoo, Finland

^b CIEMAT, Avda de la Complutense 22, Madrid, Spain

ARTICLE INFO

Keywords:

BCC crystal plasticity
Micro digital image correlation
Irradiation
Strain localization
JRQ

ABSTRACT

Capturing realistic deformation behavior in BCC metals at the polycrystal scale is an important aspect of predicting the material's strength and failure. Furthermore, local deformation/strength heterogeneity also influences the lifetime and its assessments in reactor pressure vessel (RPV) steels, especially with accumulating irradiation doses during long-term operational conditions. This work utilizes a micromorphic crystal plasticity (CP) model for BCC materials with the capability to address temperature-dependent stress-strain response and irradiation effects relevant to RPV materials. The microstructure of the investigated material was characterized prior to and during testing using electron microscopy experiments, which are used for finite element model generation and simulation result validation. To analyze the validity of the model to predict strain localization under monotonic tensile loading, micro digital image correlation (DIC) was employed jointly with the CP simulations. Different modeling choices, such as the use Schmid/non-Schmid laws and gradient based CP modeling, greatly affected the capability of the model to represent similar magnitudes in strain localization and grain reorientation. The requirement for experimental measurements, including image based analyses, on a microstructural level as a validation tool for CP modeling is clearly demonstrated.

1. Introduction

BCC metals typically display ductile fracture behavior at elevated temperatures and brittle fracture behavior at low temperatures. This is one of the most serious concerns for the pressure vessels of fission reactors and the vacuum vessels in fusion reactors. The ductile-to-brittle transition (DBT) zone is typically characterized by a transition curve and a ductile-to-brittle transition temperature (DBTT) [1].

Comprehensive investigations into failure mechanisms are essential for the development of the materials and the assessment of the mechanical integrity of components [2]. The physical mechanism of DBT is thought to be primarily governed by cleavage crack initiation and propagation. At low temperatures, brittle behaviors are usually attributed to cracks initiated at second phase particle sites. At higher temperatures, void nucleation is expected to suppress cleavage nucleation and lead to higher ductility. The fundamental mechanism underlying DBT behavior can be understood as a competition between cleavage initiation and the nucleation of ductile voids [3].

The irradiation-induced damage during service can lead to the formation of irradiation defects, such as dislocation loops and solute clusters. These irradiation defects impede the movement of dislocations,

increasing both yield stress and flow stress [4]. However, under severe loading, moving dislocations could subsequently clear and partially or completely absorb the dislocation loops, forming defect-free dislocation channels [5]. These channels are the primary cause of reduced strain hardening capacity, resulting in softening and localized plasticity. In addition to irradiation hardening, the related embrittlement is another factor that affects DBTT after irradiation [6]. The increase of flow stress caused by irradiation defects can enhance cleavage nucleation and propagation, which can explain why irradiation typically leads to an increase in the ductile-to-brittle transition temperature of structural materials [3].

Quantitative assessments of the microstructural factors mentioned above on fracture behavior are essential for integrity assessment. Existing integrity assessment methods can be divided into the global approach and the local approach. Under the global approach framework, the Master Curve (MC) method developed by Wallin and adopted in ASTM E1921, is widely employed. The application of the standard MC method is limited to macroscopically homogeneous steels with uniform tensile and toughness properties. The small-scale yielding and high constraint conditions required by the standard MC method give a

* Corresponding author.

E-mail address: matti.lindroos@vtt.fi (M. Lindroos).

<https://doi.org/10.1016/j.msea.2024.147121>

Received 13 June 2024; Received in revised form 27 July 2024; Accepted 16 August 2024

Available online 17 August 2024

0921-5093/© 2024 The Authors. Published by Elsevier B.V. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

conservative description of the fracture toughness data, but although methods have been developed to address transferability across varying levels of crack front constraints these are rather based on macroscale fracture mechanical approaches [7]. The microstructural variations in a material are also not explicitly unaccounted for. Although microstructure inhomogeneity incorporating methods have been introduced as described in Ref. [8], the resulting approaches can be insufficient in complex situations involving more realistic strain–stress states, microstructures and in accounting for different fracture modes, e.g., intergranular fracture. Therefore, it is clear that making predictions without rather extensive experimental campaigns is a complex matter.

Compared to the global approach, the local approach framework can transfer the loading conditions and microstructural variations of materials into predictions in a more direct manner [1]. The local approach establishes a link between fracture toughness and local fracture initiators, providing explicit explanations for the scatter of brittle fracture toughness related to microstructural complexity. One of the most well-known local approach models to brittle fracture was developed by the Beremin group in the 1980s [2]. However, the original Beremin-like models are oversimplified e.g., the stress value in the representative elementary volume (RVE) used for evaluation is taken to be constant. The heterogeneous nature of microstructures and induced inhomogeneous stress–strain localizations have been neglected. With advances in computing power, recent trends have been to use advanced micromechanical tools such as crystal plasticity modeling directly. This approach allows the integration of multiple microstructural factors into the prediction in an explicit way, such as crystallographic orientations, texture, grain size, and irradiation effects.

Recently, the microstructure-informed probabilistic fracture models have been developed to understand the influence of material heterogeneity on the predicted toughness [3,9–11]. These methods have demonstrated their effectiveness in determining the fracture toughness in materials by connecting microstructural features with the overall fracture behavior in terms of the modeled micromechanisms. The assessment depends on the accuracy of the stress localization predictions within the microstructure under realistic loading conditions with the used computational method. In this context, crystal plasticity (CP) provides a comprehensive framework for analyzing and predicting the micromechanical behavior of materials [12]. This framework is able to capture the behavior of various microstructures, whether they are irradiated or not, by considering factors such as grain size, morphology, defect populations (e.g., carbides [13]), and non-metallic inclusions that form during welding, which are known to affect fracture behavior by initiating cracks [14].

Different crystal plasticity constitutive models have been proposed and validated with available datasets for different RPV steel grades. The main features are comprised of either phenomenological or dislocation density based description of plasticity with irradiation defect effects with isotropic/anisotropic defect densities. For example, Vincent et al. [15] proposed a model to include irradiation effects on slip resistance and dislocation evolution to evaluate fracture probability in the spirit of the technique described in [16]. Monnet et al. [13] extended the model from this family to encompass a wider range of temperature and to introduce the evolution (and annihilation) of irradiation defects during plastic deformation. Patra and McDowell [4,17] suggested constitutive equations to define dislocation mediated plasticity in BCC with detailed evolution of defect sub-structures. This model is able to define an irradiation-induced increase in yield strength and related softening due to the annihilation of irradiation defects that leads to significant strain localization. Similar model features were proposed by Barton et al. [18] in their investigation of strain localization in polycrystalline microstructures. Chakraborty et al. [19] used dislocation dynamics informed parametrization of their model to capture yield strength and strain hardening/softening behavior in copper containing iron. The same authors [20] also utilized a cohesive zone model to investigate the ductile-to-brittle transition of RPV steels. Shi et al. [21] introduced

a mechanical damage model within a crystal plasticity framework to evaluate crack growth in polycrystals. Supporting molecular dynamics simulations have been used to define complete or partial absorption of dislocation loops to enhance irradiation defect density evolution in a crystal plasticity framework [22].

In spite of successful model behavior validation with experimental stress–strain curves, it remains uncertain whether each model is able to capture intra-grain heterogeneity during deformation, especially strain gradient effects. Image-based approaches for measuring local displacements and strains during testing can supply detailed data on the microstructural evolution during deformation. Digital Image Correlation (DIC) is one of the most prominent techniques, which has been widely employed for investigating material plasticity. DIC analyzes a sequence of images and extracts the displacements on the object surface by comparing the movement of smaller subsections throughout the image sequence. It is a versatile technique that is applicable to a wide range of length scales, and can be used to investigate objects in the micro/nano scale, provided there is a distinctive pattern or features on the object of interest. As described in the literature, this approach has been widely employed to investigate intricate phenomena involving local plasticity and material deformation mechanisms. Ghadbeigi et al. [23] were able to measure the evolution of strain partitioning between the ferritic and austenitic grains in a dual phase steel under tensile deformation, which elucidated some of the active damage mechanisms (e.g. void nucleation growth, martensite fracture, and decohesion between phases). Gioacchino and Quinta da Fonseca [24] combined μ DIC and Electron Backscatter Diffraction (EBSD) to investigate plastic straining in a stainless steel, and coupled crystallographic information with micro scale deformation to obtain a better understanding of the active deformation mechanisms. Orozco-Caballero et al. [25] investigated the deformation mechanisms and quantified the heterogeneous deformation of a magnesium alloy, reporting that local strains can be magnitudes higher on a grain level than that of the average global applied strain. Edwards et al. [26] used μ DIC to study the occurrence of twinning and slip in the lamellae of a TiAl alloy at stress below the macroscopic yield point, and reported plastic strain occurred and that it localized in softer portions of the microstructure under those conditions. Isavand and Assempour [27] were able to observe and quantify the localization of strain within narrow ferritic bands and also between lamellae during tensile testing of a ferritic-pearlitic steel. Lunt et al. [28] employed high resolution μ DIC to quantify strain localization caused by irradiation damage on relevant materials for nuclear applications.

High quality experimental data are fundamental to ensure reliable model calibration and validation, and accurately model the microstructural evolution and strain localization. Approaches combining experimental measurements in the micro scale with simulation efforts have been used by several authors. Isavand and Assempour [27] have a coupled approach that combined μ DIC and EBSD data with numerical modeling to clarify the deformation mechanisms in a ferritic-pearlitic steel. Kleinendorst et al. [29] used a connected μ DIC-FEM analysis to investigate the delamination and buckling in stretchable electronics interconnections. Lastly, the activation of slip systems and strain localization caused by degradation in harsh industrial environments was investigated by coupling experimental and computational analyses [30]. The obtained data can be used to enhance and validate material and component models used for R&D and maintenance of nuclear power plants as well as hydrogen production facilities. It is fundamental, in such engineering applications, that the behavior and life expectancy of the plant components are well understood, to assist in design and predictive maintenance efforts.

To possess at minimum adequate predictive capability on failure and fracture, the ability to describe local plasticity and related strain/stress concentrations with acceptable accuracy is of great importance. Non-local models essentially can address the effects of strain gradients, size effects, and regularize strain localization and therefore

influence on stress state. In this work, we propose a crystal plasticity model enriched with the reduced micromorphic strain gradient method [31] for unirradiated and irradiated BCC metals. The main feature is in the model's capability to regularize slip banding (strain localization) and provide size effects with a non-local framework. The model's predictive capability is evaluated with tensile experiments at different temperatures in unirradiated conditions for the so-called "JRQ" RPV steel reference material. Low-to-medium irradiation doses typical for RPV steels are investigated with the model, and compared with available experimental data at room and elevated temperatures. In addition, a numerical example is provided of a high dose case to analyze strain localization behavior. As a novelty to evaluate the predictive capabilities of the modeling approach at grain scale, deformation predictions at polycrystal level are compared with μ DIC measurements. Different modeling choices are discussed to shed light on classical CP, regularized CP, and standard Schmid and non-Schmid based CP laws.

The research paper is organized as follows. The JRQ material is initially introduced with a description of the representative volume element (RVE) generation of the investigated material, and a description of the DIC comparison related computational domain. This is followed by the details of the DIC analysis used in this work. Results are provided of the unirradiated material behavior using a 3D RVE in the simulations. Local plasticity simulations are presented and compared with DIC datasets using a quasi-3D microstructure with different modeling approaches, including standard Schmid's law model, different micromorphic variables, and a non-Schmid model variant. Corresponding model errors and the capability to present lattice re-orientation are discussed. Then, irradiated conditions are investigated with the model using the 3D RVE to assess the stress-strain response validity. Finally, sensitivity analysis is performed with quasi-3D DIC computational domain with irradiation defects to analyze dose effects on strain localization.

2. Materials and methods

2.1. Material

An ASTM A533 grade B class 1 reference RPV steel, known as JRQ, was used for the investigation described in this work. This material was initially determined as a reference RPV material by the International Atomic Energy Agency (IAEA) in 1983 [32]. It has been widely investigated and is sensitive to irradiation embrittlement, displaying a considerable increase in hardness and yield strength with irradiation [33]. More general information on its thermomechanical properties and chemical composition can be found at [32]. Fig. 1 shows an optical microscopy characterization of JRQ's microstructure with Nital etching, and further microstructural details of this material can be found in the Refs. [34–37].

Miniature tensile specimens were prepared using electrical discharge machining (EDM) from JRQ blocks that were available at VTT Technical Research Centre of Finland. These dog bone specimens were prepared with a gauge length of 0.5 mm, a 1 mm width at the reduced section, and 0.5 mm thickness. The specimens were prepared for imaging by mechanical grinding followed by polishing using a VibroMet 2 vibratory polisher. Further details on the specimen geometry and surface preparation are described in Ref. [38]. Two distinct tests were carried using the in-situ system and the miniature specimen, one under optical microscopy to obtain stress-strain data and investigate the strain distribution in the specimen under tensile load, and another monitored with scanning electron microscopy (SEM) to carry out measurements on the microstructural level up to a specific strain level within the range of uniform deformation. In the first test, load was measured using the in-situ testing system and DIC was used as an optical extensometer to measure displacement in the gauge portion of the specimen up to failure. For the second test, a microindentation device

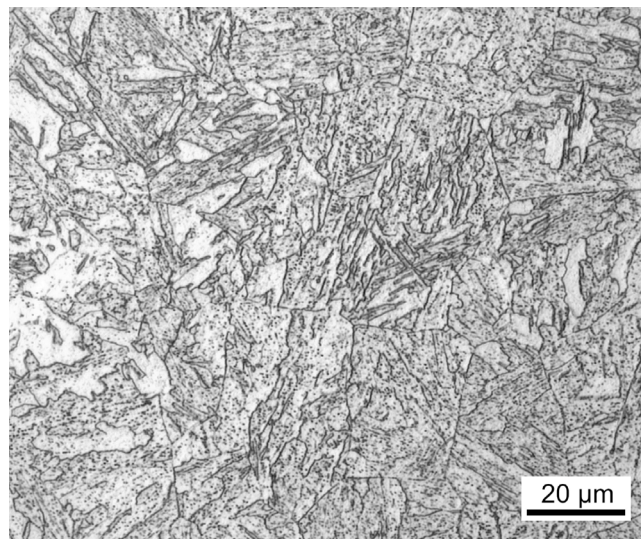


Fig. 1. Light optical microscopy image of JRQ material depicting its microstructure after etching with 3% Nital solution for approximately 30 s.

was used to demarcate the area-of-interest within specimen with four indents using 30 mN of force to delimit a region of approximately 250 by 250 μ m which would be investigated with SEM during mechanical testing. The area between the indents was investigated with Electron Backscatter Diffraction (EBSD) prior to and after testing using a SEM Zeiss crossbeam 540 with a EDAX Trident (EDS-EBSD-WDS) system. Fig. 2 depicts the overlapped inverse pole figure (IPF) and image quality (IQ) maps, the kernel average misorientation (KAM) map obtained from the EBSD analysis, as well as the scanning electron microscopy image showing the carbide distribution in the undeformed JRQ specimen. The initial microstructure of the material is composed mostly bainite with sparse ferritic islands, with a grain size of 3.2 ± 2.5 μ m, and a fine carbide with a mean diameter of 0.073 ± 0.07 μ m dispersed throughout the microstructure. The EBSD analysis shows a microstructure with no preferential crystallographic orientation, and KAM map shows a microstructure with a misorientation of roughly 2° , with plate like regions with practically no misorientation. KAM is related to local geometrically necessary dislocations (GNDs) and the observed pattern is in accordance with that which would be expected from a bainitic microstructure [39].

A miniature pneumatic bellows loading device was used to carry out the in-situ tensile tests of miniature specimens both under optical microscopy and inside a Zeiss Ultra Plus SEM. This is a custom-made system designed to allow mechanical testing inside an SEM with accurate measurements of load and displacement. This system uses pressurized gas to control the movement of the pneumatic loading unit, and a self regulating loop guarantees the test parameters set by the user. The displacement of the specimen is measured using a Linear Variable Differential Transformer (LVDT) sensor, while the load is calculated based on the pressure inside the bellows, the stiffness of the bellows, and its cross-sectional area. The coupling of mechanical testing data with SEM imaging, and ex-situ EBSD analysis allows the simultaneous investigation of the material's mechanical response and microstructural evolution. An extensive description of this experimental setup and its applications is available in Ref. [38]. The in-situ tensile device applied two deformation levels to the miniature specimen, with global axial strain values of 1.4% and 5.4%, respectively, at strain rates of approximately 0.5×10^{-4} s^{-1} . Considering that a minor stress relaxation is observed once a given displacement is applied and kept constant, imaging of the area of interest was only started once the load signal is fully stabilized after approximately 5–10 min.

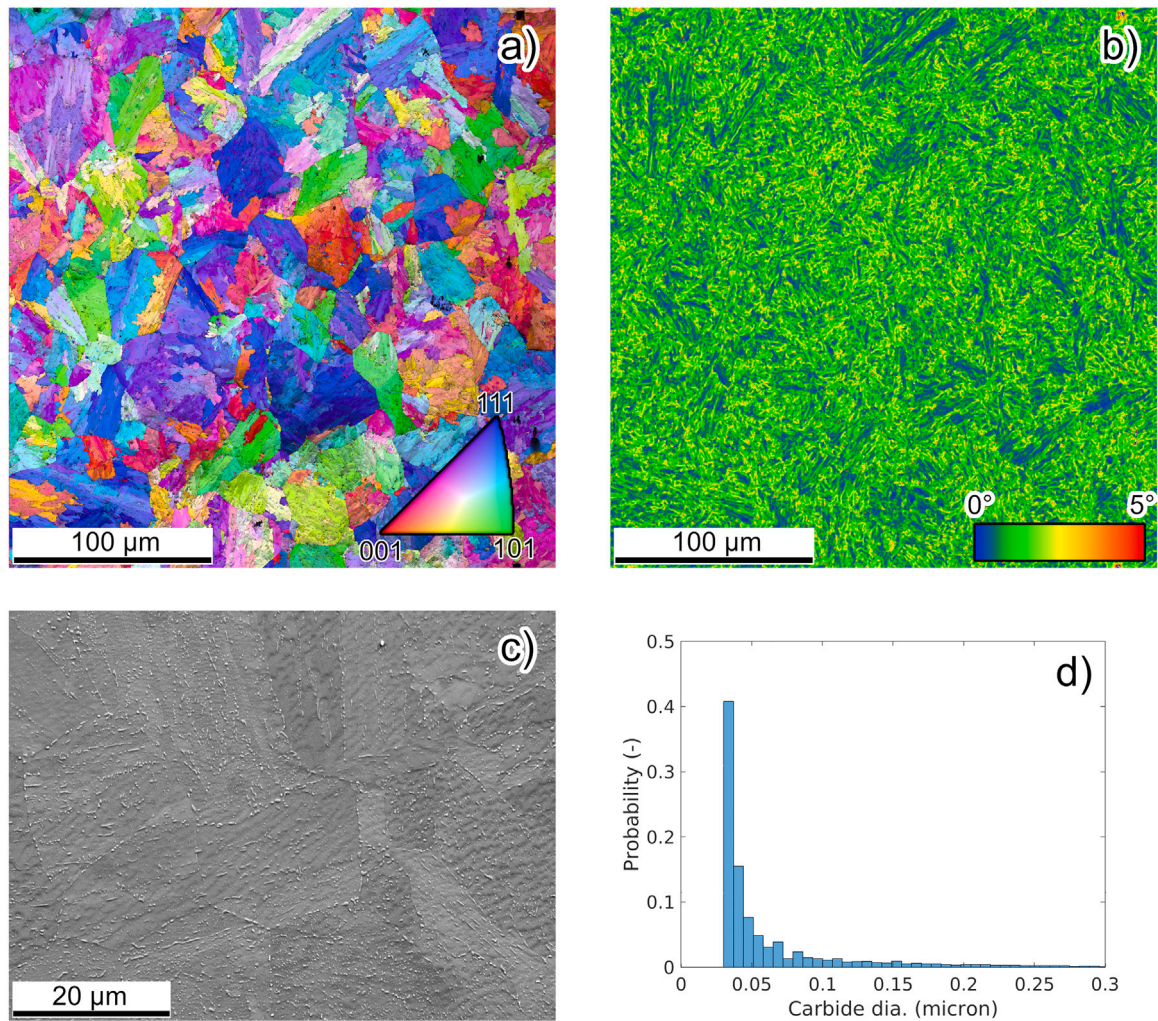


Fig. 2. EBSD (a) inverse pole figure (IPF)/image quality (IQ), (b) kernel average misorientation (KAM) maps of undeformed JRQ specimen, and (c) scanning electron microscopy image of JRQ material and (d) histogram of the equivalent diameter of the observed carbide particles.

Additionally, the models in this work also utilize results of previous tensile tests carried out at temperatures ranging from 123 to 673 K from unirradiated and irradiated material provided by ÚJV Řež (referred as dataset Exp1-x) and Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT) (referred as dataset Exp2-y) [40].

2.2. Digital image correlation on a microstructural level

Acquisition of SEM images of the region-of-interest between the indents during the in-situ test was carried out using the secondary electrons detector (SE2) and an accelerating voltage of 5 kV. Image acquisition in the SEM was automated for high magnification images to be taken in a grid-like manner to cover the whole area. A grid of 9 by 10 images was taken for each deformation step, with a resolution of 4096 by 3072 pixels, an 11 nm/pixel scale, and a 20% overlap. The relative positioning between each image and overlapping of the acquired images for each step was carried out using the Grid/Collection stitching function [41] within the Fiji image analysis platform [42]. The properly aligned images were then merged using Enblend 4.2 [43,44], an open source plugin that employs the Burt-Adelson multi-resolution spline approach [45] to blend composite images together, taking into account the features in the overlapping regions to obtain the best possible seam between images. The resulting image after the overlapping and merging process for the non-deformed specimen is shown

in Fig. 3. Given that the final output image is not a perfect square, and that the lower indents are almost out of the field of view, it is clear that some level of drifting occurred during the automated imaging of the area. This problem was mitigated by selecting a larger area of interest than that demarcated by the indents. Additionally, it is clear that undesired carbon contamination by the electron beam occurred during imaging, which appears as the dark shaded square in the image. Although there was an initial concern about increasing contamination over several imaging steps, this ended up having a negligible effect on the DIC analysis, which already accounted for the different ranges of gray between images. While preparing the merged images for DIC analysis, they were initially manually post-processed, so that the canvas of the images would have the exact same image resolution and the upper right corner would be roughly in the same position.

DIC was initially carried out using only the topmost right image of each step to verify the feasibility of microstructural features as a pattern, and to set initial analysis parameters. A smaller area was used for the initial optimization, as using full-sized images would have been too computationally time consuming. Subsequently, the parameters that led to the best results were used to analyze images of the whole area of interest, and the analysis took about three days of computation. The parameters used in the μ DIC analysis are described in detail in Table 1. The following full-field quantities of interest were extracted from the DIC analysis: x-displacement, y-displacement, axial strain,

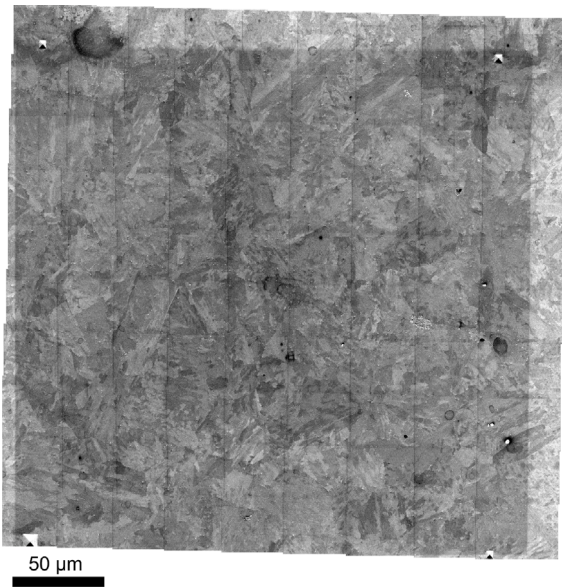


Fig. 3. High magnification secondary electron SEM image for large analysis area obtained with automated grid imaging, stitching and merging.

Table 1
μDIC hardware and analysis parameters.

Microscope	Zeiss Ultra Plus SEM
Image resolution and digitization	27975 by 27419 pixel ² , 8 bit
Field-of-view	307 by 301 μm ²
Detector	Secondary electrons (SE2)
Image scale	0.09 pixel/nm
Working distance	13.5 mm
Patterning technique	Carbide distribution and microstructural features
Carbide size distribution	14 ± 6 pixels // 0.073 ± 0.07 μm
DIC Software	LaVision DaVis 10.2.1
Total number of images	3
Speckle quality [46]	6.07
Subset size	137 pixels // 1.50 μm
Step size	41 pixels // 0.45 μm
Strain window	13 data points
Virtual strain gauge size	629 pixels // 6.9 μm
Correlation mode	Sum of differential
Shape function	Affine
Weighting function	Round (Gaussian)
Matching criterion	Weighted variables-based sum of squared differences (WVBSSD)
Interpolant	7-tap B-spline function
Strain formulation	Engineering

transverse strain, and shear strain. The results of the analysis were post-processed to remove any clear outliers based on a threshold for the correlation value and residuals of the DIC vectors.

Rigid transformations (translations and rotations) that were not caused by the deformation of the material were removed from the vector field. Considering that DIC analysis was done on merged composite images with slightly different image sizes, shifts in the image position would be recognized by the algorithm as translation, even if it would not be related to the actual displacement of the specimen. Nevertheless, rigid body motion does not affect the strain calculations, considering that the strain analysis is based on the relative displacement between subsets. Fig. 4 shows the comparison between the obtained full-field displacement map prior to and after the rigid body transformation. The displacements on the upper right of the original displacement field are close to zero, as the images were aligned according to that indent. Displacements grow and have different directions towards the other edges. The displacement field without rigid body transformation has roughly no displacements in its center of mass, and displacements

grow symmetrically towards the edges. The vertical contraction and horizontal extension of the microstructure are clearly visible from the displacement arrows in the transformed displacement field, which was not as evident prior to the removal of the rigid body movement.

The full-field results from the μDIC analysis support the crystal plasticity modeling efforts in two distinct ways: (1) it provides high resolution strain maps of the microstructure for validation of the modeling results; (2) it provides accurate displacement information on the boundaries of the area-of-interest which can be used to set the boundary conditions. Ultimately, these results are most impactful when further combined with crystallographic data from the investigated material. The next subsection describes the application of EBSD and SEM data to generate representative quasi-3D and full 3D virtual microstructures that were used with the crystal plasticity modeling approaches.

2.3. Microstructure characterization and digital twin

To digitally simulate experiments, a statistically representative virtual microstructure of the material that captures its microstructural features is required. These virtual microstructures are referred to as representative volume element (RVE) and they were generated in the current work using the following steps. The Greninger–Troiano (G–T) orientation relationship [47] is used to reconstruct the prior austenite grains (PAG) in the EBSD data (shown in the left of the Fig. 5), with the crystallographic texture of the reconstructed PAG being random. In the center of Fig. 5 the correlation between the PAG size with the number of martensite packets and blocks is shown, the axes have been max-normalized. It indicates that larger PAG consists of more martensite packets and variants. The generation of the 3D digital twin of the microstructure is performed using Neper software [48], which begins with the prior austenite RVE (shown in top right corner of the Fig. 5), using the grain size distribution and the orientations obtained from the PAG reconstruction of the EBSD data. Using the correlation between the PAG size and the packets/blocks, the number of packets and blocks are estimated for each PAG in the RVE, which is then used to generate the bainite RVE (shown in the right corner of Fig. 5).

In the following step, a quasi-3D finite element mesh is generated from the EBSD map. The domain is discretized with 400 by 400 quadratic C3D20R elements with reduced integration. This yields an element edge size of approximately 560 nm. The physical size of the rectangular computational domain is 225.73 × 225.73 μm. Special boundary conditions are applied based on the displacement data of the same region in the DIC experiment. Sixth degree polynomial fits are made for each edge of the computational domain to match the spatial axial displacements from DIC displacement data. The back side of the domain is fixed in Z-direction, while a free surface is retained for the front side. The model is clearly a simplification of the real condition, and no information is available of the subsurface grain structure. This is expected to generate errors in the simulations, as noted also in [49]. Fig. 6 shows the applied boundary condition and the computational domain with the grain structure. A total of 8064 different orientations/grains were included in the computational domain, which results from the two degree misorientation threshold in defining element sets as grains.

2.4. Crystal plasticity model

The following section describes the crystal plasticity model for the unirradiated and irradiated material. The present model shares many features with the model proposed by Monnet et al. for BCC containing irradiation defects [13], and in this work, we further extend it with a micromorphic reduced strain gradient method [31]. Additionally, irradiation induced solute clusters are also included in the model, and the effect of dislocation loops and their interactions was evaluated.

Finite strain formalism is used with the decomposition of the deformation gradient to elastic and plastic contributions $\underline{F} = \underline{F}^E \cdot \underline{F}^P$.

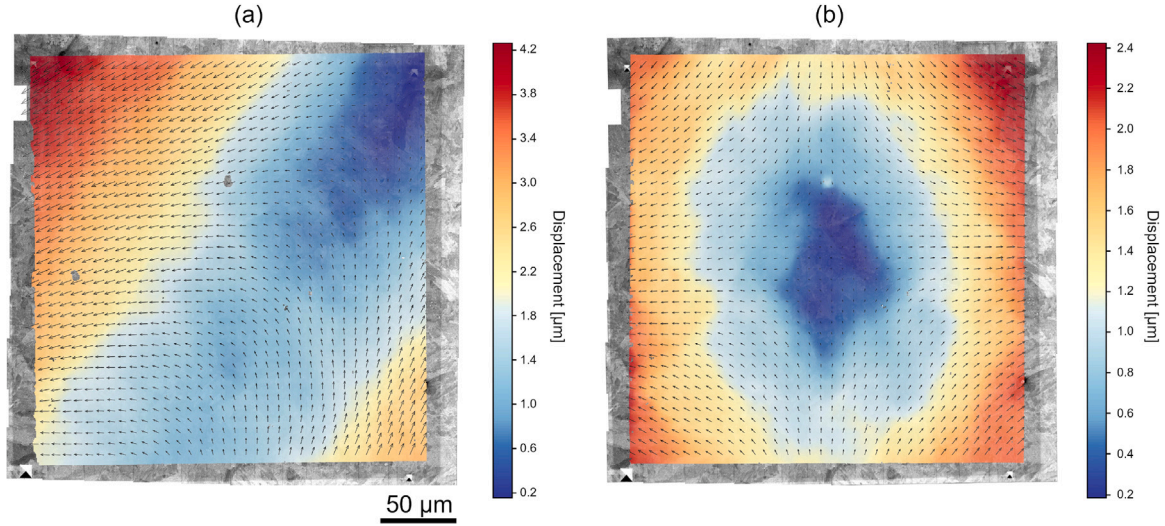


Fig. 4. (a) Original and (b) rigid body motion corrected full-field displacement maps of the microstructure at a global strain of 1.4%. The color map describes the amplitude and the black arrows the direction of the displacement. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

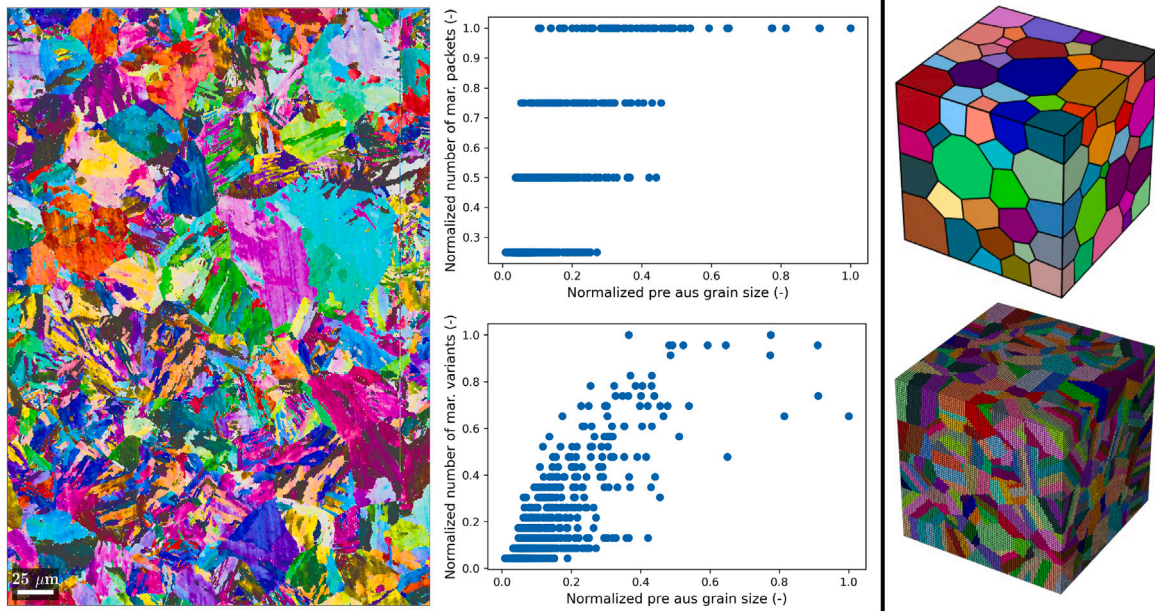


Fig. 5. Electron backscattering diffraction IPF map with the statistical correlation between the prior austenite size and the number of child martensite packets/variants. The corresponding generated RVE of the prior austenite as well as the child martensite.

The plastic velocity gradient is defined as $\underline{L}^P = \sum_{s=1}^{N_s} \dot{\gamma}^s \underline{S}_0^s$, where $\underline{S}_0^s$ is the orientation tensor of a slip system s . The slip rate is defined as a harmonic sum of slip rates required to nucleate kink pairs, and on the other hand, to subject enough driving force for jog drag. The two contributions are denoted by drag and lattice friction terms.

$$\frac{1}{\dot{\gamma}^s} = \frac{1}{\dot{\gamma}_{drag}^s} + \frac{1}{\dot{\gamma}_{friction}^s} \quad (1)$$

A viscoplastic formulation (power-law) is chosen for the jog drag mechanism for each slip system s . The slip rate contribution $\dot{\gamma}_{drag}^s$ is defined:

$$\dot{\gamma}_{drag}^s = \dot{\gamma}_0 \left[\frac{|\tau^s|}{\tau_c^s} \right]^n \text{sign}(\tau^s) \quad (2)$$

where $\dot{\gamma}_0$ is the reference strain rate, τ_c^s is the shear resistance, parameter n defines strain rate sensitivity, and τ^s is the resolved shear stress

on system s . An alternative model with enrichment using non-Schmid terms is described later at the end of this section, which modifies the computation of τ^s . The shear rate for the lattice friction regime is given as the conventional thermally-activated dislocation motion [50] by:

$$\dot{\gamma}_{friction}^s = \rho_m^s b^s H l_{sc}^s \exp \left(-\frac{\Delta G}{kT} \left(1 - \left[\frac{\tau_{eff}^s}{\tau_0^s} \right]^p \right)^q \right) \text{sign}(\tau^s) \quad (3)$$

where ρ_m is mobile dislocation density (set constant here), b^s length of Burgers vector, H jump frequency, l_{sc} is the average length of screw dislocation segments, k is the Boltzmann constant, T is the absolute temperature, ΔG is activation energy, and τ_0^s is the lattice resistance of each slip family, considered different for $\{110\}$ systems, system family $\{112\}$ twin directions and $\{112\}$ anti-twin directions. An effective stress

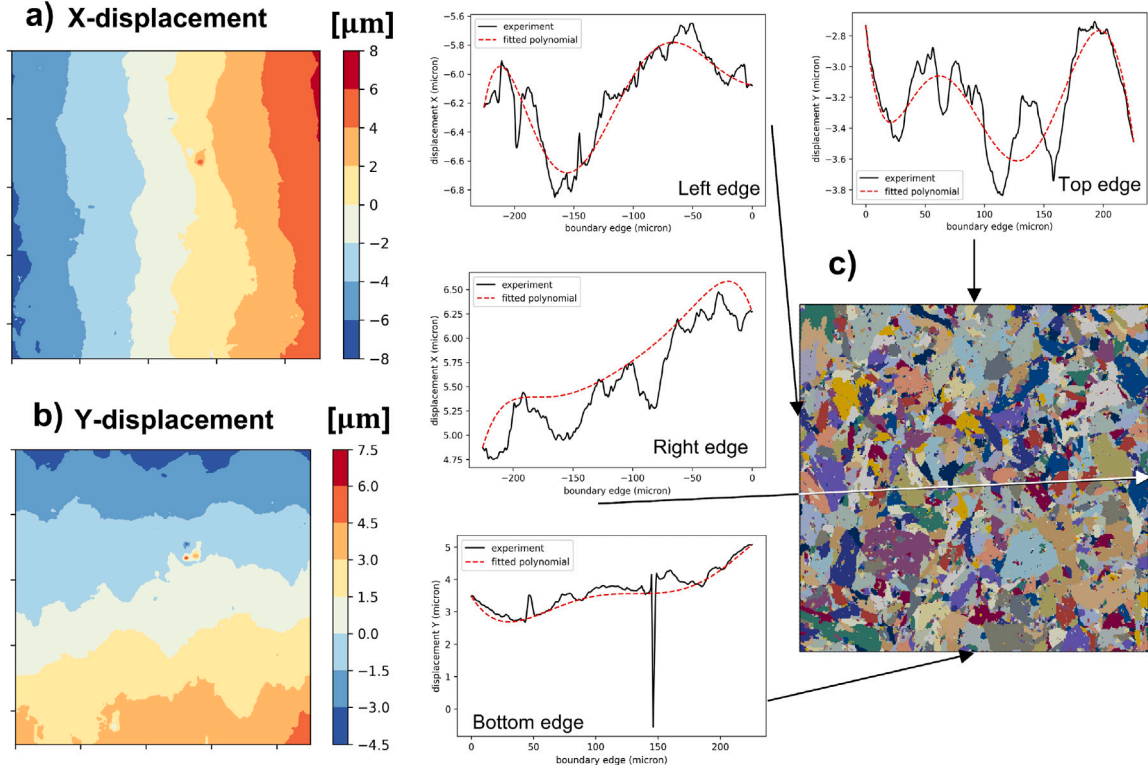


Fig. 6. Boundary conditions and microstructure for EBSD based computational domain, (a) horizontal axial DIC displacement field, (b) vertical axial DIC displacement field, (c) FE computational domain with grain structure and boundary conditions.

τ_{eff} is defined as the mean stress driving dislocation motion.

$$\tau_{eff} = \begin{cases} |\tau^s| - \tau_c^s, & \text{if } |\tau^s| > \tau_c^s \\ 0, & \text{otherwise} \end{cases} \quad (4)$$

Slip resistance τ_c^s is considered generally as a combination of solid solution strengthening, grain size (Hall-Petch) effect, self and line tension hardening contributions. The solid solution strength is considered small for lowly alloyed materials. In the current model we include this effect in the Hall-Petch contribution, i.e., $\tau_{0/SS}^s$ is set zero as an individual term.

$$\tau_c^s = \sqrt{(\tau_{self}^s)^2 + (\tau_{LT}^s)^2} + \tau_{HP} + \tau_{0/SS}^s - S_\chi \quad (5)$$

where τ_{self}^s is self hardening contribution, τ_{LT}^s is line tension contribution, τ_{HP} Hall-Petch term. Generalized stress is introduced in the spirit of reduced micromorphic framework $S_\chi = -H_\chi(\gamma_{cum} - \gamma_\chi) = A\Delta_\chi\gamma_\chi$ [31]. An additional degree of freedom is considered related to microslip γ_χ . Cumulative plastic slip is defined as $\gamma_{cum} = \int_0^t \sum_{i=1}^{N_s} |\dot{\gamma}^s| dt$. Two length-scale parameters are then introduced H_χ and A . As a major difference of the previous and current modeling approaches, the current model is dislocation density based including irradiation defects that influence on temperature dependent stress-strain state predictions and most importantly on the strain localization behavior in the presence of irradiation defects. Therefore, the known capability of the micromorphic part of the model [31] to regularize strain localization is adopted within the current framework.

The Hall-Petch contribution is provided by:

$$\tau_{HP} = \frac{\mu}{\mu(RT)} \frac{K_{HP}}{\sqrt{d_{bcc}}} \quad (6)$$

where μ is shear modulus at a given temperature, $\mu(300 \text{ K})$ shear modulus at 300 K reference temperature, K_{HP} is the Hall-Petch constant at 300 K, and the effective grain size is estimated with d_{bcc} . The definition of effective grain size in martensitic/bainitic steels is non-trivial and controversial to define, whether to relate it to either packet, block or

lath size, or the mean value of the aforementioned. We utilize effective grain size defined from the EBSD map, as discussed in Section 2.3.

Self slip resistance is expressed as

$$\tau_{self}^s = \mu b^s \sqrt{a_{self} \rho^s} \quad (7)$$

The present model utilizes the line tension contribution proposed in Ref. [13], where more details can be found related to the effectiveness of this model choice.

$$\tau_{LT}^s = \max \left[\frac{\alpha^s \mu b^s}{\lambda^s - l_c} - \tau_{eff}, 0 \right] \quad (8)$$

where α^s is the mean obstacle strength coefficient, parameter l_c is the minimum length of screw segment, λ average obstacle spacing, and τ_{eff} the effective stress defined in Eq. (4). It should be noted that this line tension model will regain the classical Taylor's formulation at high temperatures, and when the average obstacle spacing approaches $1/\sqrt{\rho_{obs}}$, so that $\tau_{LT}^s = \alpha^s \mu b^s \sqrt{\rho_{obs}^s}$. A planar density expression ρ_{obs}^s is used:

$$\rho_{obs}^s = \sum_{s \neq j} \rho_{dis}^j + \rho_{carb} + \rho_{SC} + \rho_{DL} \quad (9)$$

where carbide defect density is introduced with $\rho_{carb} = C_{carb} D_{carb}$, and C_{carb} D_{carb} are the average carbide number density and size, respectively. RPV steels have a high population of submicron carbides, which will cause a significant Orowan type of hardening. Irradiation related defect densities are denoted with ρ_{SC} and ρ_{DL} for solute clusters and dislocation loops, respectively. These defect densities will be discussed in the following in more detail.

Solute clusters

Irradiation induced solute clusters are found highly relevant for strengthening RPV materials [51]. Monnet et al. introduced an additional solute cluster defect density to influence flow stress and dislocation density evolution. The defect density ρ_{SC} can be expressed with [13]:

$$\rho_{SC} = C_{SC}^s D_{SC}^s \quad (10)$$

where C_{SC}^s is the planar number density and D_{SC}^s the average size of the clusters. Solute clusters can be sheared by dislocations and effective reduction in their pinning effect is established with [13]:

$$\dot{C}_{SC}^s = -\lambda_{SC}^s \frac{D_{SC}^s}{b^s} C_{SC}^s |\dot{\gamma}^s| \quad (11)$$

where parameter λ_{SC}^s is used to describe the magnitude of the annihilation process of solute clusters. Effectively, the initial solute cluster planar density and average size are assigned equal to all slip systems in spite that the model formulation essentially tracks the evolution of each planar density depending on the activity of slip on that slip plane.

Dislocation loop model I: Monnet et al. [13] proposed a dislocation loop model that considers one type of loop density that equally contributes to the hardening of each slip system, similar to the model formulation of solute cluster defects. Dislocation loop defect density is expressed:

$$\rho_{DL} = C_{DL} D_{DL} \quad (12)$$

where dislocation loop number density is C_{DL} and D_{DL} is the average size of loops. It is taken that dislocation loops can then be annihilated/absorbed during plastic slip, and the annihilation rate is given by:

$$\dot{C}_{DL}^s = -\lambda_{DL}^s \frac{D_{DL}^s}{b^s} C_{DL}^s |\dot{\gamma}^s| \quad (13)$$

where λ_{DL}^s determines the magnitude of annihilation/absorption, ranging generally between zero and one. No distinction is made between the active slip system and loop type, and therefore all active slip systems contribute to the annihilation depending on their effective slip rate.

Dislocation loop model II: Alternatively, Barton et al. [18], and Chakraborty and Bulent Biner [19] used a tensorial interaction between the loop type and dislocation slip system. Anisotropic interaction between dislocations and $1/2\langle 111 \rangle$ and $\langle 100 \rangle$ loops are distinguished in this defect description. The defect density is modified to:

$$\rho_{DL} = \underline{N}^s : \underline{H} \quad (14)$$

where $\underline{H}$ is a second order defect tensor. Interactions between the loops and slip systems are incorporated in a defect tensor formulation, where the slip plane normal tensor is defined as $\underline{N}^s = n^s \otimes n^s$.

$$\underline{H} = \sum_i 3N_{DL} d_L^i (\underline{I} - n_i^i \otimes n_i^i) \quad (15)$$

where N_{DL} is the initial number density of a loop type, and d_L is the average size of loops or given size distribution distributed in the microstructure. Loop plane normals are denoted with n_i^i .

The evolution of the irradiation (damage) tensor is given by:

$$\dot{\underline{H}} = -\eta \sum_s (\underline{N}^s : \underline{H}) \underline{N}^s |\dot{\gamma}^s| \quad (16)$$

where η determines the magnitude of annihilation/absorption in this model. No particular upper limit is set for the value. However, generally it can be set between 0 and 200, where 200 can already generate a significant local softening after a small amount of local dislocation slip. The model does not account for loop size dependent annihilation separately [52], which can address the size distribution of loops and their absorption. It should be noted that the most restrictive aspect of the model is often the unknown distribution of dislocation loops over different planes. In spite of this restriction, the dislocation loop model II is used in the current work.

Irrespective of which of the dislocation loop models is used, the average obstacle strength is estimated as a function of various defect densities.

$$\alpha^s = \frac{1}{\sqrt{\rho_{obs}^s}} \sqrt{\sum_{s \neq j} a_{eff}^{sj} \rho_{dis}^j + a_{carb} \rho_{carb} + a_{SC} \rho_{SC} + a_{DL} \rho_{DL}} \quad (17)$$

where a_{eff}^{sj} is the interaction matrix between dislocation slip systems. Evolving dislocation interaction coefficients are employed [13].

$$a_{eff}^{sj} = \left(0.2 + 0.8 \frac{\ln(0.35b^s \sqrt{\rho_{obs}^s})}{\ln(0.35b^s \sqrt{\rho_{ref}^s})} \right)^2 a^{sj} \quad (18)$$

where a^{sj} are the constant values for the interactions. ρ_{ref} is a reference total dislocation density, in which the interaction constants are determined, effectively set to $1 \times 10^6 \text{ 1/mm}^2$ in this work following [13].

An average obstacle spacing is defined in the model to conform with low and high temperature ranges.

$$(\lambda^s)^{-1} = \min[\sqrt{\rho_{obs}^s}; D^s \rho_{obs}^s] \quad (19)$$

where curvature diameter of non-screw dislocations is approximated with $D^s = \mu b^s / \tau_{eff}^s$.

Evolution of dislocation density is related to the mean free path. Different self and obstacle contributions are defined for multiplication.

$$\dot{\rho}^s = \frac{|\dot{\gamma}^s|}{b^s} \left(\frac{1}{d_{bcc}} + \left(1 - \frac{\tau_{eff}^s}{\tau_0^s} \right) \left(\frac{\sqrt{a^{self} \rho^s}}{K_{self}} + \frac{\sqrt{a^s \lambda^s \rho_{obs}^s}}{K_{obs}} \right) - y_s \rho^s \right) \quad (20)$$

where K_{self} and K_{obs} describe the average number of self and obstacle interactions of dislocation before immobilizing. To simplify, a relationship of $K_{obs} = K_{self}/3$ is adopted here. It should be noted, that τ_0^s refers to the critical shear stress of a slip family that is considered different, i.e., $\{110\}$, $\{112\}$ TW twinning direction and $\{112\}$ ATW anti-twinning directions [13]. The annihilation distance in the original model is defined as:

$$\frac{1}{y_s} = \frac{1}{G_{cc}} + \frac{2\pi \tau_{eff}^s}{\mu b^s} \quad (21)$$

where G_{cc} is the annihilation distance constant, that dominates the annihilation process at high temperatures.

More distinctive control strain rate and temperature dependency can be applied [53]. We apply this definition of the annihilation distance in this work.

$$y_s = 2G_{cc} \left(1 - \frac{K_b T}{A_{rec}} \ln \left| \frac{\dot{\gamma}_0^s}{\dot{\gamma}_0^s} \right| \right) \quad (22)$$

where reference slip rate is defined accordingly as $\dot{\gamma}_0 = \rho_m^s b^s H I_{sc}^s$, which is usually in the range of $1.0 - 5.0 \times 10^7$. Parameter A_{rec} is effectively used to scale temperature and strain rate dependency on annihilation distance.

GND density is estimated from the norm of microslip vector $\mathbf{K}$ in the reduced micromorphic model [54]:

$$\rho_{GND} = \|\mathbf{K}\|/b^s \quad (23)$$

Non-Schmid model extension

As a model alternative to the conventional definition of Schmid based resolved shear stress τ^s , the effect of non-glide stresses is introduced. We utilize the three-term non-Schmid modification for the resolved shear stress [53,55]. Hence, the resolved shear stress computation from the conventional $\tau^s = \underline{M} : \underline{S}_0^s$ is modified with three non-Schmid parts so that $\tau^s = \underline{M} : (\underline{S}_0^s + w_1 \underline{S}_{NS1}^s + w_2 \underline{S}_{NS2}^s + w_3 \underline{S}_{NS3}^s)$. Weight factors for non-glide stresses are denoted by w_1 , w_2 , and w_3 . Only slip family $\{110\}\langle 111 \rangle$ slip systems are operational in this model, containing 24 slip systems due to asymmetry.

$$\underline{S}_{NS1}^s = \mathbf{m}_0^s \otimes \mathbf{n}_0^s \quad (24)$$

$$\underline{S}_{NS2}^s = (\mathbf{n}_0^s \times \mathbf{m}_0^s) \otimes \mathbf{n}_0^s \quad (25)$$

$$\underline{S}_{NS3}^s = (\mathbf{n}_0^s \times \mathbf{m}_0^s) \otimes \mathbf{n}_0^s \quad (26)$$

where $\mathbf{m}_0^s$ is the slip direction and $\mathbf{n}_0^s$ is the slip plane normal of a slip system s . Plane normal $\mathbf{n}_0^s$ has an angle of 60 degrees to the primary slip plane $\mathbf{n}_0^s$. The non-standard slip plane normals and slip directions are listed, for example, in [53] and not repeated here.

3. Results and discussion

In this section, the stress–strain response of the model is compared with experimental datasets in unirradiated conditions at different temperatures. The RVE constructed in Section 2.3 is used for the analyses. Irradiation defects are introduced and the model response is compared against experimental stress–strain behavior. Subsequently, low-to-medium dose levels are primarily analyzed and also compared to experimental tensile test results. This is followed by a comparison of deformation localization using μ DIC measurements and model predictions using different modeling approaches based on the same EBSD map measured of the surface of the tensile specimen within the region of interest for the unirradiated material. Finally, irradiation defects are introduced in the same EBSD based computational domain to perform a sensitivity analysis on their effect on strain localization with the model.

3.1. Stress–strain behavior at different temperatures

The model parameters are adjusted to correspond to the material tensile behavior at 123 K, 183 K, 297 K and 563 K. This serves as the baseline model parameter identification also for later sensitivity analyses. In general in Fig. 7, the model predictions agree well with the experimental datasets. Two different experimental datasets were used, which are denoted by Exp1-x and Exp2-y, where x and y are the numbering of the individual tests. Exp1-x dataset is more consistent with a number of tests showing very similar material behavior, while Exp2-y dataset shows more variations.

The model does not predict the observed distinctive yield point effect, especially at low temperatures 123 K and 183 K. From the modeling point of view, this is due to the absence of any back-stresses in the microstructure initial condition or any specific model to address dislocation avalanche after micro-yielding (e.g., dynamic strain aging model). However, the model is satisfactorily capable of predicting strain hardening of the material beyond the initial yield point affecting up to ten percent of strain. Beyond this point, it is assumed that the necking of material will play an influential role in the experiments, which is not aimed at capturing the used RVE approach with kinematic uniform boundary conditions. Furthermore, no damage model [31] is activated in the present approach which could already influence the saturation of stresses near the peak strength of the material.

At room temperature, taken as 297 K here, the model overestimates strain hardening compared to the experimental dataset Exp1-x slightly. On the other hand, the variations in the Exp2-y dataset indicate that the model prediction is within the range of error for the material stress–strain response. Furthermore, the room temperature stress–strain curve obtained using a miniature specimen in the in-situ system under optical microscopy is also in good agreement with the model prediction. At high temperatures (563 K), the model matches the material's yield point well. While the strain hardening response is more limited than observed in dataset Exp1-x, it is still within the margin seen in Exp2-y.

Fig. 8 illustrates Von Mises stress and dislocation density distributions for 123 K and 563 K cases. Elevated stress state is observed generally for the 123 K case throughout the microstructure in compared to 563 K temperature. It is observed that 563 K still shows high stresses in the grains and grain boundary regions that are found also hotspots at 123 K in spite the average Von Mises stress of the RVE is lower at 563 K. A plate-like stress distribution is observed for the 123 K at stress levels of 600–700 MPa, which mostly smoothens out when temperature increases. The simulation results at both temperatures show dislocation densities above $1 \cdot 10^{15} \text{ m}^{-2}$ in the regions having stress hotspots at regions such as grain boundaries. However, smoother spatial distribution is observed for the 123 K case, highlighting less pronounced dislocation accumulation at specific grain boundaries in the microstructure in compared to 563 K simulation.

Table 2 lists the identified model parameters. These parameters are used for the basic part of the model without irradiation defects in the

Table 2
Model parameters.

Description	Symbol	Value	Unit
Elastic constant	C_{11}	236.0	[GPa]
Elastic constant	C_{12}	134.0	[GPa]
Elastic constant	C_{44}	119.0	[GPa]
Shear modulus	μ	$(236 - 0.0459T)/2.6$	[GPa]
Reference slip rate (power law)	$\dot{\gamma}_0$	5.0×10^{-5}	[s ⁻¹]
Strain rate exponent	n	50.0	[–]
Length of Burgers vector	b^s	0.248	[nm]
Activation energy	ΔG	2.25×10^{-19}	[J]
Energy barrier parameter	p	0.32	[–]
Energy barrier parameter	q	1.15	[–]
Minimum segment length	l_c	5.0	[nm]
Mobile dislocation density	ρ_M	1.0×10^7	[1/nm ²]
Initial dislocation density (total)	ρ_0	1.68×10^8	[1/nm ²]
Reference dislocation density	ρ_{ref}	1.0×10^7	[1/nm ²]
Frequency factor	H	2.0×10^{11}	[s ⁻¹]
Hall–Petch coefficient	K_{HP}	3.9525	[MPa/ $\sqrt{\text{mm}}$]
Effective grain size	d	3.5	μm
Solid solution strength	$\tau_{0/SS}$	0.0	[MPa]
Self hardening parameter	K_{self}	18.0	[–]
Obstacle hardening parameter	K_{obs}	$K_{self}/3$	[–]
Dislocation interaction	a_i	0.7 collinear, others 0.1	[–]
Thermal resistance 110	τ_0^{110}	360.0	[MPa]
Thermal resistance 112TW	τ_0^{112TW}	410.0	[MPa]
Thermal resistance 112ATW	τ_0^{112ATW}	480.0	[MPa]
Reference annihilation distance	G_{cc}	$1.5 \times b^s$	[nm]
Capture radius energy	A_{rec}	4.5×10^{-20}	[J]
Average carbide size	D_{carb}	73.0	[nm]
Number density of carbides	C_{carb}	2.38×10^{20}	[1/m ³]
Carbide interaction	a_{carb}	1.0	[–]
Length-scale penalty	H_x	5000 and variable	[MPa]
Length-scale parameter	A	0.005 and variable	[Nmm ²]
Non-Schmid weight ^a	w_1	0.3	[–]
Non-Schmid weight ^a	w_2	0.1	[–]
Non-Schmid weight ^a	w_3	0.05	[–]

^a Indicated separately if non-Schmid behavior is used

following sections. In principle, as the drag term of the model will become dominant at high temperatures, the model fit could be improved by modifying the drag part of the model to be more temperature dependent. For example, reference slip rate $\dot{\gamma}_0$ and strain rate exponent n could be set as a function of temperature [56,57]. However, this was not attempted in this work and a single set of parameters is retained for all temperatures. The main fitting parameters of the model are initial dislocation density ρ_0 that influence yield of the material, hardening variable K_{self} (K_{obs} is related to K_{self}) that influences strain hardening capability in irradiated material, reference annihilation distance G_{cc} that controls strain hardening and saturation, and A_{rec} that influences on strain rate and temperature dependency of annihilation distance. Other parameters such as carbide strengthening related to its defect density and irradiation defect densities (solute clusters and dislocation loops) are aimed to be defined from experimental/characterization data, and therefore are not exactly used as fitting parameters. However, we use defect density interaction coefficients a_{SC} and a_{DL} partially as fitting parameters, but limited to a range reported in literature. Additional non-local effect on hardening is attributed to parameters A and H_x , which are used to regularize slip localization in the current work.

3.2. Irradiated material behavior

RPV materials generally experience relatively low doses during their operational lifetime. In the following, we evaluate how the model is able to predict the material's tensile behavior in irradiated conditions with low to medium doses (<1 dpa).

The material was populated with irradiation-induced solute cluster and dislocation loop defect densities, utilizing Eqs. (10) and (12). Two different fluence ranges are investigated. Table 3 lists the used

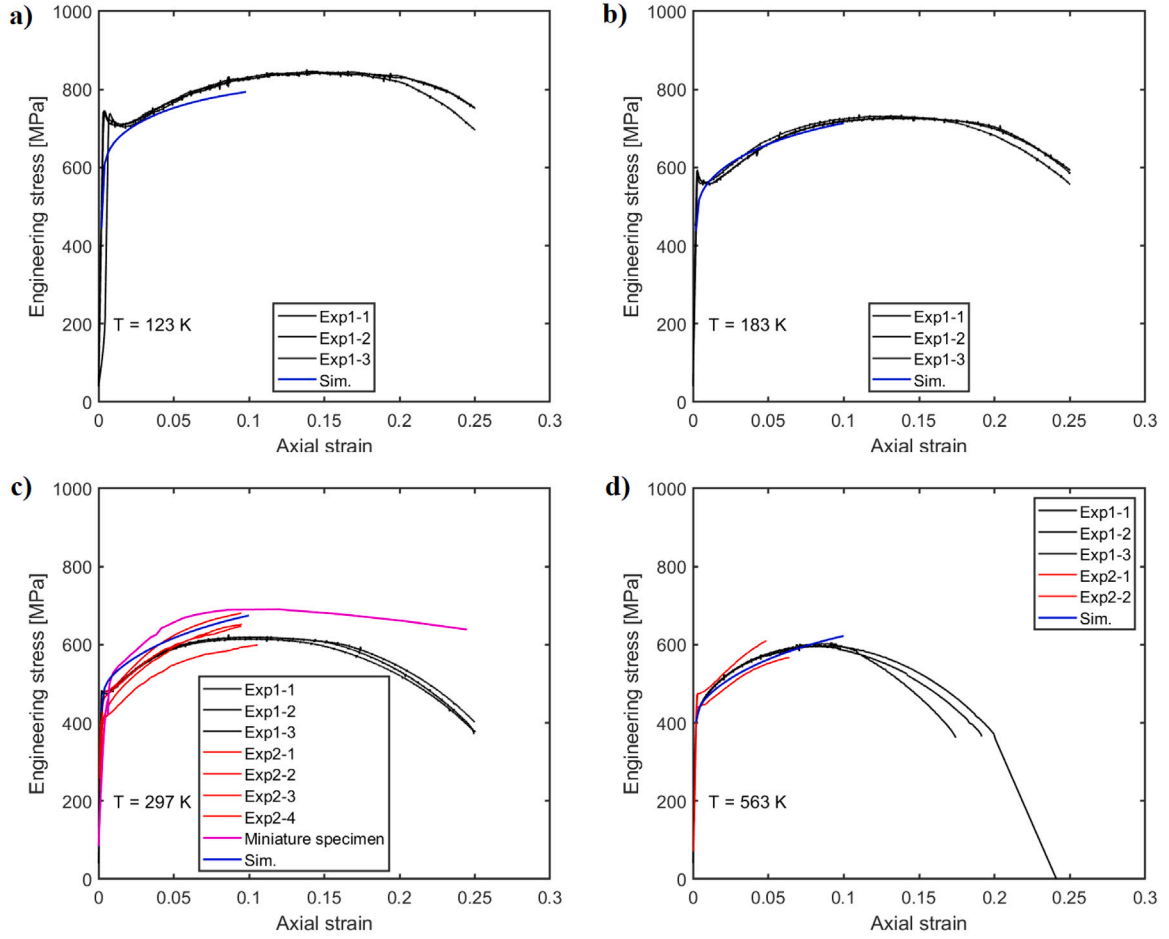


Fig. 7. Experimental and simulated stress-strain curves at (a) 123 K, (b) 183 K, (c) 297 K (room temperature), (d) 563 K (290 °C).

parameters for the simulations. A correlation of $1.0 \text{ dpa} \approx 6.67 \times 10^{20} \text{ n/cm}^2$ is used [58] to estimate displacement per atom for reference. Experimental data consisting of stress-strain curves at room and elevated temperatures originated from two different data sources, denoted again by Exp1-X and Exp2-Y. The reported fluences range from $1.56 \times 10^{18} \text{ n/cm}^2$ to $30.0 \times 10^{18} \text{ n/cm}^2$.

Dislocation loop densities and average sizes are reported for JRQ in [59] for fluence $4.2 \times 10^{19} \text{ n/cm}^2$ (flux $0.28 \times 10^{12} \text{ cm}^{-2} \text{ s}^{-1}$, $E > 1 \text{ MeV}$) and for $4.0 \times 10^{19} \text{ n/cm}^2$ (flux $1.6 \times 10^{12} \text{ cm}^{-2} \text{ s}^{-1}$, $E > 1 \text{ MeV}$) to be $C_{DL} = 3.19 \times 10^{21} [1/\text{m}^3]$, $D_{DL} = 3.18 \text{ nm}$ and $C_{DL} = 1.0 \times 10^{21} [1/\text{m}^3]$, $D_{DL} = 3.18 \text{ nm}$, respectively. The average size of the loops does not show significant change due to fluence, however, the neutron flux can influence the loop number density. Hence, we choose lower dislocation loop number density for lower fluences in the simulations and slightly higher for the higher fluences.

Dislocation loop density was set for [100] type loops. Loop density on [111] was set to zero, since if the density in all [111] planes is equal, the off-diagonal terms will be canceled in the reconstruction of loop damage tensor H (Eq. (15)). Dissimilar loop densities on each plane can be assigned, however, no experimental data is available to support these choices for the investigated material. Moreover, for similar material like EUROFER97 ferritic-martensitic steel, studies report conflicting results regarding loop distribution on habit planes, with some having observed DLs mainly on [100] planes and some on [111] planes [60]. Solute cluster shearing parameter λ_{SC}^s was set to 0.4 and dislocation loop annihilation parameter η was set to 20.0 using the dislocation loop model II. Solute cluster interaction parameter a_{SC} was set to 0.02, rendering smaller, but still notable, additional slip resistance. Similarly low values, 0.03 and rather negligible, have been reported

Table 3

Model parameters of irradiated condition ($1.0 \text{ dpa} \approx 6.67 \times 10^{20} \text{ n/cm}^2$) [58].

Low dose I				
Fluence	$4.4 \times 10^{18} \text{ n/cm}^2$	0.0066 dpa	Exp-1 dataset	
Fluence	$3.64 \times 10^{18} \text{ n/cm}^2$	0.0055 dpa	Exp-2 dataset	
Model parameters				
Description	Symbol	Value	Unit	
Solute cluster number density	C_{SC}	1.0×10^{23}	$[1/\text{m}^3]$	
Solute cluster average size	D_{SC}	1.5	[nm]	
Dislocation loop number density	C_{DL}	1.0×10^{21}	$[1/\text{m}^3]$	
Dislocation loop average size	D_{DL}	2.75	[nm]	
Medium dose II				
Fluence	$1.56 \times 10^{19} \text{ n/cm}^2$	0.0234 dpa	Exp-1 dataset	
Fluence	$3.0 \times 10^{19} \text{ n/cm}^2$	0.045 dpa	Exp-2 dataset	
Model parameters				
Description	Symbol	Value	Unit	
Solute cluster number density	C_{SC}	2.0×10^{23}	$[1/\text{m}^3]$	
Solute cluster average size	D_{SC}	1.5	[nm]	
Dislocation loop number density	C_{DL}	2.5×10^{21}	$[1/\text{m}^3]$	
Dislocation loop average size	D_{DL}	3.19	[nm]	

for EUROFER97 steel [61,62]. Dislocation loop interaction parameter a_{DL} was set to 0.18. For similar steel materials a wide range between 0.17 [63] and 0.68 [61] has been reported. Identical initial dislocation density was retained in all simulated cases for simplicity. The same 3D RVE described in Section 2.3 was used in these simulations.

Fig. 9a–c shows the simulated and experimental tensile stress-strain curves in irradiated condition for temperature 297K with two

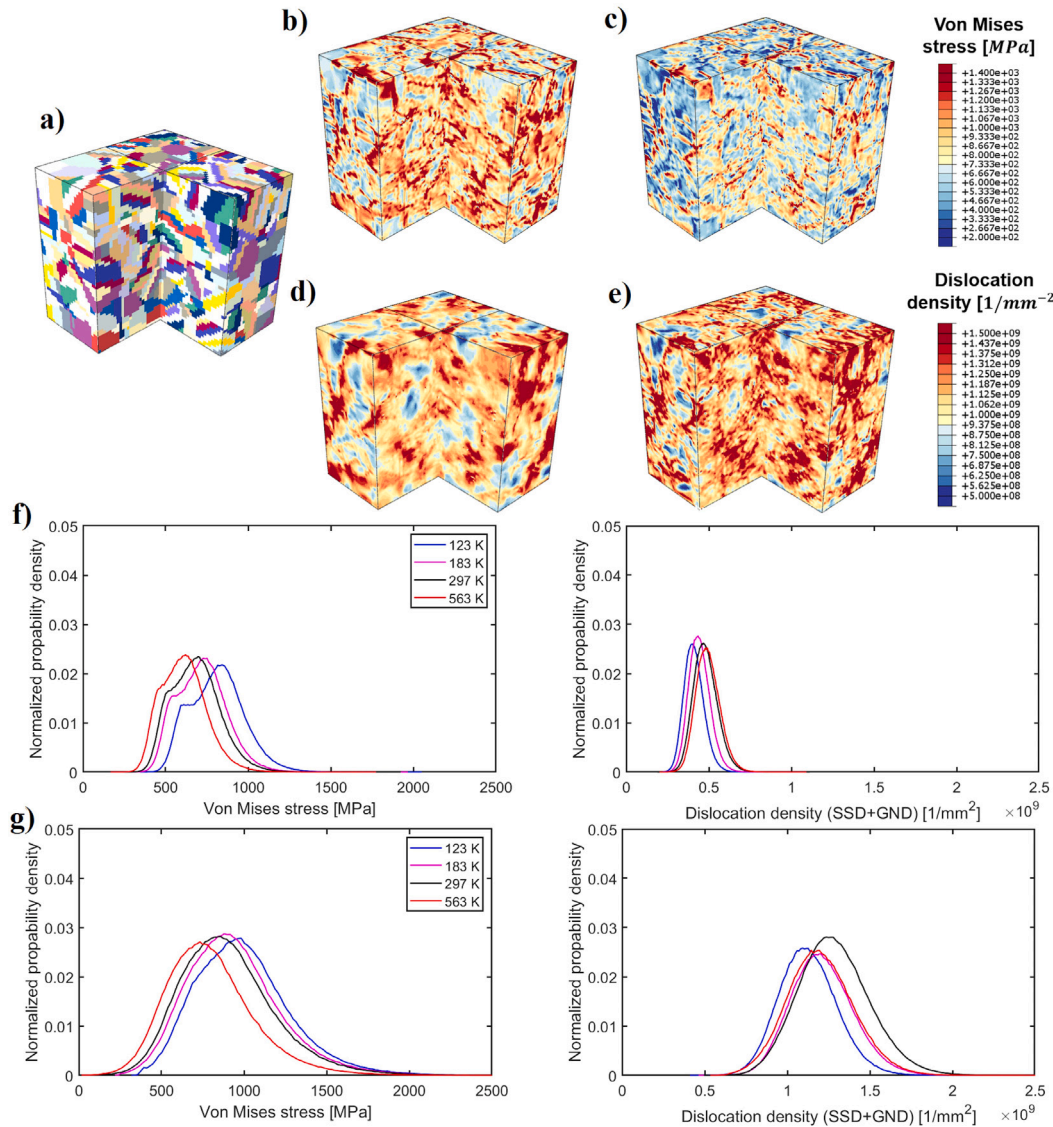


Fig. 8. (a) RVE used for simulations, von Mises stress for (b) 123 K and (c) 563 K, dislocation density for (d) 123 K and (e) 563 K. Probability density distributions of von Mises stress and dislocation density at (f) 2.5% of axial strain and (g) 10% of axial strain.

fluences (Dose I and II) and for temperatures 563K and 673K (Dose I) based on two different experimental datasets. The model reproduces the low dose (Fig. 9a and d) well. Higher dose level (Fig. 9b and e) introduces more uncertainty in the predictions. Exp2-Y dataset is quite well in agreement, while it is observed that Exp1-X dataset is underestimated by 8%–9% using the same model parameter set for both cases. The prediction on Exp1-X dataset could be improved by assigning higher irradiation-related defect densities, which would lead to higher apparent yield stress of the material in the model. However, no particular characterization data is available of the average defect densities or defect sizes between the used datasets (the fluence range is very similar) to justify the selection.

Model response at higher temperatures is again two-fold (Fig. 9 c and f). Simulated yield stress correlates with the experimental yield stress in dataset Exp1-X. However, significantly lower predictions are observed for Exp2-Y dataset. The 673 K experimental curve yields at around 500 MPa, which is very similar to the room temperature yield stress of about 490–510 MPa. Hence, it is inevitably expected that the model predicts a much lower yield point due to the temperature dependency in the model. Furthermore, the sole high temperature curve does not allow for evaluating deviations in the experimental data as is observed in cases tested at room temperature.

Two methods of addressing gradient enhanced hardening/softening are presented with simulated blue and red curves. The red curve (sim.) follows the original model with a possibility for the generalized stress S_χ to impose additional hardening or softening. The blue curve (sim. hard) defines a situation where S_χ is enforced to produce only hardening ($S_\chi > 0$). Artificially enforcing only hardening leads to improved approximations in some of the stress–strain responses, while in other cases overestimation is observed. If the original model is used with softening and hardening effect, the strain hardening rate is suppressed with the irradiated material condition, while the unirradiated model predictions in Fig. 7 are in satisfactory agreement. This indicates that the additional hardening term can be too restrictive in either way, using hardening only or softening/hardening with irradiation influenced material. In contrast to the recent work of Abatour and Forest [64], the current model does not use saturating variables. This aspect then remains a topic for possible improvement in the current model. Overall, it is observed that model predictions are mostly in line with the experimental results, given a 5% error margin, and the aforementioned observations related to higher temperature(s).

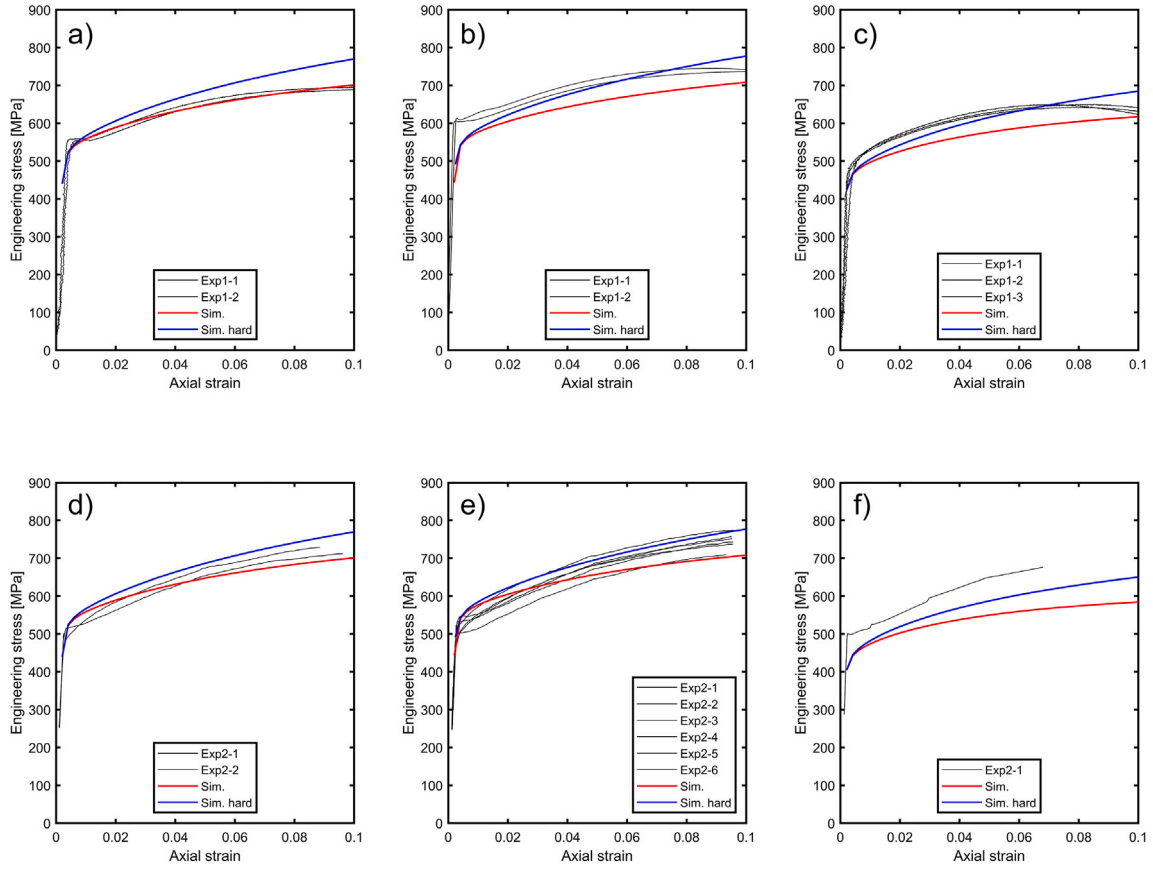


Fig. 9. Tensile stress–strain curves of irradiated material, Exp-1 dataset: (a) low dose I at 293 K, (b) medium dose II at 293 K, (c) low dose I at 563 K. Exp-2 dataset: (d) low dose I at 293 K, (e) medium dose II at 293 K, (f) low dose I at 673 K. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3.3. Comparison of local deformation of DIC and models

A comparison of the local strain field is made between experimental DIC data and crystal plasticity simulations. Fig. 10 shows the comparison of horizontal, vertical, and shear strains. Different simulation cases were investigated, consisting of two regularized cases with different micromorphic length-scale parameters, a local crystal plasticity case, and regularized non-Schmid cases with different length-scale parameters. We compare the DIC measured and simulated strain maps at a global horizontal axial strain of approximately 5.4%. The DIC fields in Fig. 10 displays the uncorrelated regions and removed outliers as white, which are not considered in the comparison. Qualitatively, the local strain fields appear largely similar, which suggests that the simulations and experimental data are correlating well pattern-wise. Discrepancies are seen in some grains showing either higher or lower deformations in the most dominant horizontal strain field.

Regularized Schmid's law based and non-Schmid models - Fig. 10b,e - show smoothing of the local strain magnitudes in compared to the classical local crystal plasticity simulation in Fig. 10d. This is especially observed for the low length-scale parameters $H_\chi = 5000$ MPa and $A = 0.005$ N mm². Higher local magnitudes appear when the length-scale parameters are adjusted more tightly to avoid diffusive spread coming from the regularization with $H_\chi = 50000$ MPa and $A = 0.001$ N mm². With these parameters, the model response is becoming more similar to the standard local crystal plasticity case. It should be noted that the local crystal plasticity is expected to overestimate local strains in general. To highlight the local strains in Fig. 10, the strains legend is restricted with the limits shown in the figure. This masks some of the highest local strains when using the local CP approach.

Mesh sensitivity analysis is performed in Appendix B. The gradient approach shows an almost mesh-insensitive solution for the horizontal

strain field, while the local crystal plasticity is more mesh dependent. The von Mises stress distribution is also less mesh-sensitive with the gradient model. However, full mesh independence is not established stress-wise in either case. Appendix C shows the size dependent scaling of the standard Schmid's law model. Saturation of flow stress is established with decreasing size of microstructural characteristics (grain size), as expected from the non-local model.

Full-field maps provide an appropriate qualitative overview, but despite strain values being displayed in different colors, a direct quantitative comparison is complicated. We quantified, therefore, the difference in strain magnitude between simulations and experiments using probability density plots. Additionally, the L1 error ($= \sum_i |f^{exp}(g_i) - f^{sim}(g_i)|$, where f^{exp} and f^{sim} are the probability density functions from experiments and simulations results, respectively) was computed to show the cumulative difference between simulation and experimental results. Fig. 11a–c show the probability distributions of local strains. This confirms visual analyses in Fig. 10. The strain distributions from simulations adequately match those from the experiment. The scalar L1-norm (Fig. 11d–f) presents the cumulative difference between the experiment and simulations.

Oversmoothing is evident for the standard Schmid's law based micromorphic regularized simulation with low H_χ and high A values. The prediction is improved with the choice of different length-scale parameters. Based on the L1-error, non-Schmid model correlates also well irrespective of the choice on length-scale parameters for the dominant horizontal strains. A good correlation is found for the local CP model in the horizontal strain values, but it does not show any improvement of the other modeling choices for vertical and shear strains. Also, the local CP model experiences very high local strain hotspots, which is masked out in the comparison. The quantitative comparison in Fig. 11

plots all material point level data but does not provide information of spatial correlation visually presented in Fig. 10. Therefore, no definite judgment on the superiority of each method can be established based on the L1-error alone.

Obtaining adequate spatial correlation between the EBSD crystallographic data and full-field data from the SEM images can be an intricate challenge. Four indentation marks were used as anchor points to select the same analysis area for both datasets. However, there are experimental obstacles that make it complex to obtain a perfect correlation. The EBSD analysis required a long analysis time, which makes it susceptible to drifting of the specimen over time. Moreover, it visualizes the specimen at a 70° angle, which is addressed by a geometric correction of the viewing angle. On the other hand, SEM images were taken at a perpendicular angle. However the image acquisition also took considerable time and is prone to drifting, lens distortion, and inaccuracies introduced by the merging procedure. While the adequate spatial correlation was obtained, it is plausible that there is a horizontal shift of even up to tens of microns between the experimental and modeled datasets. Nevertheless, based on our visual analysis, the non-Schmid model does not provide particularly improved predictions when compared with the standard Schmid's law, given the obtained resolution with the DIC measurements.

Appendix A includes a comparison of the experimental DIC and simulated strain fields for the lower axial strain of approximately 1.4%. Visual comparison of the strain fields shows a slightly better correlation. However, probability density analysis shows a similar range in the error between experiments and simulations using different models. Therefore, it can be stated that the model predictions do not improve or degrade with increasing strain in the sample, at least in the studied strain range.

We consider several reasons for the local differences between experiments and simulations. Firstly, the current model approach does not account for explicit micron sized or submicron carbides in the computations, which could influence local strain states by suppressing or activating different slip systems. Secondly, we utilize constant initial dislocation density throughout the microstructure. Assignment of heterogeneous distribution could potentially improve localization behavior, for example, as defined with KAM or related GND distribution in Fig. 2. Thirdly, the model is based on quasi-3D approach with unknown subsurface grain structure, which is expected to influence the outcome of the simulations.

Fig. 12 shows the comparison of IPF plot of the deformed microstructure observed in the experiments (Fig. 12a) and simulations. Three simulation cases are selected, namely the local crystal plasticity model (Fig. 12b), regularized CP $H_x = 50000, A = 0.001$ (Fig. 12c), and non-Schmid regularized CP $H_x = 50000, A = 0.001$ (Fig. 12d). Two sub-regions containing a few grains are chosen for this highlighted comparison (cutout windows are magnified 2.2\times), which are labeled as [1] and [2] in the figure. The following observations can be distinguished:

1. The grain reorientation in the local CP model is stronger in comparison to other simulation methods, as indicated by the sharper contours in the IPF plot.
2. The grain reorientation in the local CP model is closest to the experiments in spite of occasional high local strain hotspots.
3. In the grain [1] for the non-Schmid case there is some missing reorientation at the bottom of the grain, whereas the grain [2] has additional reorientation. The addition of slip family $\{112\}\langle 111 \rangle$ might be necessary to generate reorientation similar to the experiments.

While the local crystal plasticity model results agreed with the experiments well, the simulations showed very high stress/strain spikes, which could influence the prediction of crack nucleation and as an overall indication can lack physical justification. Therefore we propose

that local regularization should be considered in order to avoid extensive localization in strains or stresses, as any predictions for failure essentially depend on these values, either with a full crystal plasticity formulated damage model, or post-processing based models. For example, Ren et al. used the Microstructure Informed Brittle Fracture (MIBF) model to predict fracture properties of RPV steel microstructures [11]. To eliminate extremely high local stress and include grain morphology effects, it was proposed simply that local scale stress fields are averaged on the smallest structure to assess brittle crack penetration, such as a bainitic packet in bainitic steel. The current results indicate that this could be possibly established directly with a well-behaving non-local model, but the validity of each model should be performed with means of local strain analysis such as the μ DIC approach used in this work.

4. Local scale plasticity analysis of irradiated material

As a numerical example, we investigate different irradiated conditions at a low tensile strain (5.4%) with the EBSD based model described in Section 2.3. First, a medium dose range with dislocation loop density of $C_{DL} = 4.0 \times 10^{21}$ and average size of $D_{DL} = 4.0$ nm is investigated to analyze irradiation effects on strain localization with the proposed model. Solute cluster annihilation is retained at $A_{SC} = 0.4$ and the loop annihilation parameter is kept at $\eta = 20.0$. A high dose case with loop density of $C_{DL} = 6.9 \times 10^{21}$ and average size of $D_{DL} = 6.1$ nm [60] is also given for the sake of a numerical comparison. To demonstrate the localization behavior with irradiation, we also define a higher dislocation loop annihilation rate for the highest dislocation loop defect case, i.e., $\eta = 50.0$.

Fig. 13 shows total dislocation density, GND density approximated with Eq. (23), von Mises stress of each studied case, and a comparison of the stress-strain response of each case. Both dislocation density and stress state are elevated from the unirradiated state. However, it is observed that the model does not predict very significant changes in local plasticity from unirradiated to medium dose cases. Dislocation density is increased locally and some banded regions can become more populated with dislocations and therefore appear thinner. A similar trend is observed in the von Mises stress state in terms of localization.

Overall, stresses are elevated with the presence of irradiation defects, as expected due to the introduction of additional defect densities. A high dose combined with a high dislocation loop annihilation rate shows very significant strain localization, which is also reported by [4, 18] with a similar kind of dislocation loop model. The dominant shear bands predicted by the model involve high dislocation density and secondary bands that are formed in the in-between regions. Other zones in the material show less deformation due to the existing shear bands with concentrated deformation. This outcomes from reduced slip resistance during the reduction of dislocation loop density, which promotes formation of localization bands. Effectively, these areas can also be interpreted as bands clear of dislocation loops [65] exactly because the loop defect density has significantly decreased.

The current model with micromorphic regularization could be used to control such shear bands. Fig. 13b shows the approximated GND density caused by plastic deformation. GNDs evolve around slip rich regions (high dislocation density in Fig. 13a). This is shown in the high dose simulation, where GND accumulation is observed bordering the apparent shear bands because of the strong gradient in microslip. In effect, this regularizes the thickness of the slip rich or shear band regions. However, validity of the method to produce finite sized bands is uncertain without actual validation measurements from a test specimen with a high irradiation dose. The stress-strain curves in Fig. 13d show a qualitative difference between the simulated cases with a quasi-3D microstructure. It is observed that the higher dislocation loop density and related annihilation show reduction in the strain hardening rate. As pointed out in Section 2.3, the quasi-3D meshes can underestimate the stress-strain response of the material due to the often used plane strain/stress assumption, which leads to lower overall flow stress predictions in compared to Fig. 9. Even so, the model effectively predicts changes in the localization and strain hardening behavior of the material at various dose levels.

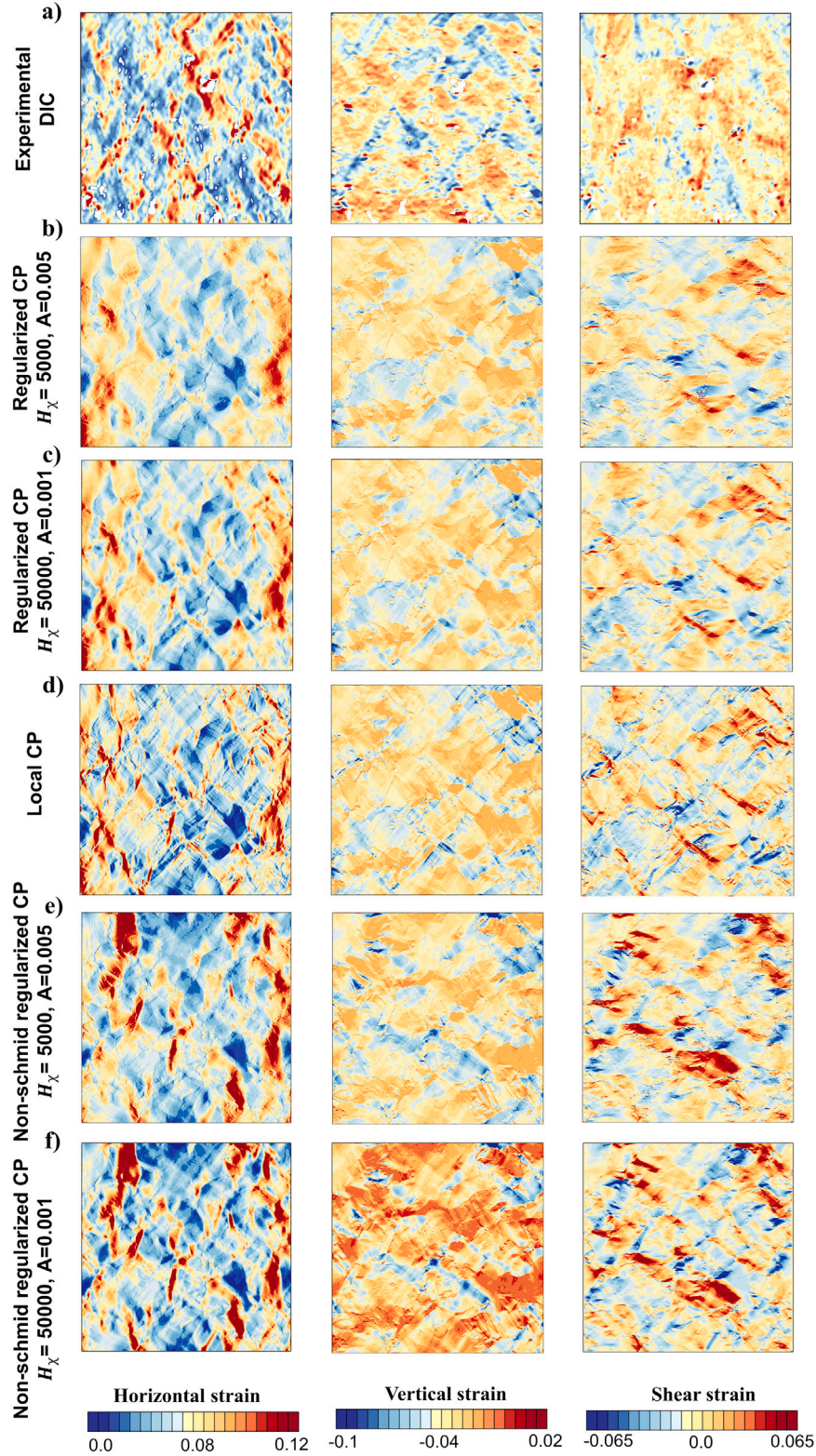


Fig. 10. DIC experimental and simulated horizontal, vertical and shear strain fields, (a) experimental μ DIC strain fields, (b) regularized non-local plasticity with $H_x = 5000$ MPa and $A = 0.005$ N mm², (c) regularized non-local plasticity with $H_x = 50000$ MPa and $A = 0.001$ N mm², (d) local crystal plasticity, (e) Non-Schmid regularized non-local plasticity with $H_x = 5000$ MPa and $A = 0.005$ N mm², (f) Non-Schmid local plasticity with $H_x = 50000$ MPa and $A = 0.001$ N mm² at a global horizontal strain of circa 5.4%. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

5. Restrictions of the approach and future aspects

Carbides are treated non-explicitly only as a defect density and average size is prescribed. This choice neglects any sub-micron scale

stress and strain concentrations around the carbides. Overall, as improved data becomes available either from experimental sources or multiscale modeling workflows, the use of distributed values for the defect structure is preferred. This is an important aspect if any damage

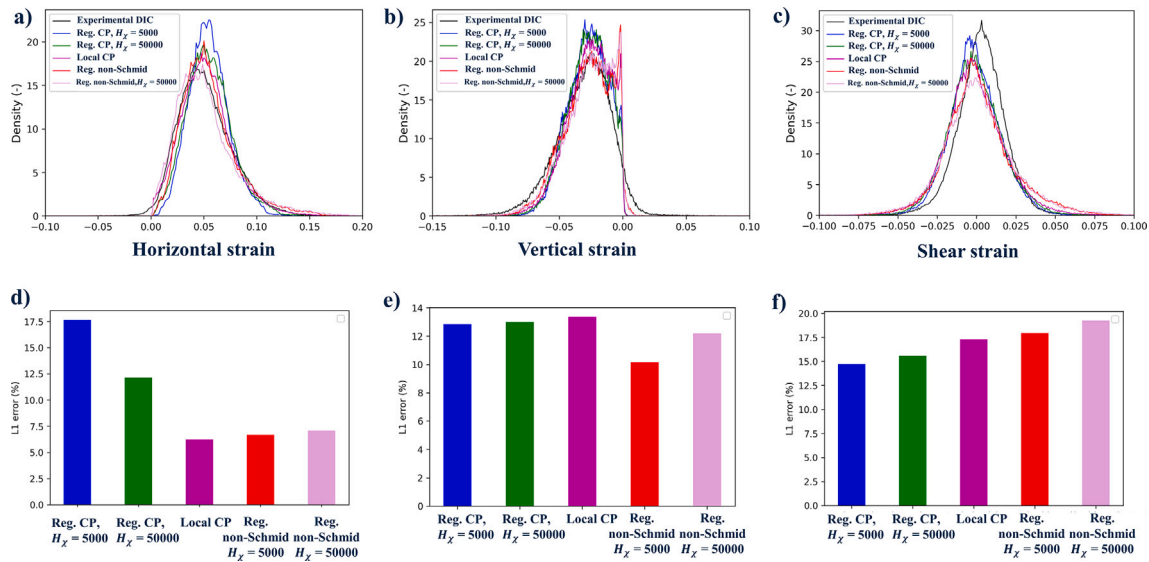


Fig. 11. Probability density plots of (a) horizontal strain, (b) vertical strain, (c) shear strain, and the respective error bars (d)–(f).

model is involved [14]. The crystalline cleavage damage model could be used in the framework [31]. This type of model, however, assumes that damage is described on specific (cleavage) planes and no direct ductile fracture behavior is involved, unless the model parametrization is devoted to temperature dependent and ductile-like sluggish crack growth. At present the current model does not account for mechanical damage for these reasons. Li et al. [66] suggested a mixed model for FCC material to address different damage mechanisms. Similarly for FCC, phase field damage modeling offers a coupling to plastic work as a contributor to the fracture driving force [67] to imitate more ductile like behavior with fundamentally brittle behaving phase field model. In all of these cases, a care should also be placed on the regularization of strain and damage fields represented at the level of the microstructure and the nature of fracture mechanism. Alternatively, the validated model behavior in this work allows more robust use of so-called microstructurally informed brittle fracture models [11]. This approach enables users to utilize plasticity results and couple them with a probabilistic model to predict failure and shifts in the ductile-to-brittle master curve. It should be noted that we discuss mechanical damage (explicit cracking), not to be confused with irradiation damage, which remains a future topic. Furthermore, the model does not include vacancy formation constitutes explicitly or dislocation climb model in the current form, which is demonstrated important for high temperature creep behavior [68,69].

The current work does not cover μ DIC validation of local plasticity in irradiated conditions. Therefore, the model predictions of irradiated material local scale plastic localization should be considered speculative, given the available data on the investigated material. Furthermore, even higher spatial resolution in μ DIC would be required to enable the validation of model behavior at finer length scales, e.g., of finite thickness of slip bands. Overall, the μ DIC method used in this work must be further refined. Higher magnifications and finer patterns on the specimen would be required to obtain experimental strain measurements of phenomena such as the formation of slip bands and deformation twins. The analysis of larger areas of interest containing more grains and more deformation steps would also provide a more representative description of the microstructural evolution of the material throughout deformation. As stated, the current work does also not introduce explicit carbides in the microstructure, for example, sub-micron carbides that were observed largely in the JRQ material. Tests with model alloys are also expected to support the development of the experimental techniques and partition the contributions arising from different microstructural features. Data on the location, size, and shape

of precipitates could be obtained from the same initial overview of the microstructure that is used as the reference image for μ DIC. In such efforts, an excellent spatial synchronization with the data obtained from imaging and EBSD would be required for the modeling approach to include precipitate information. Such simulations at the level of large 3D polycrystal would be computationally costly with the present model. Furthermore, the current modeling approach did not include heterogeneity in initial dislocation density based on approximation of GND density from EBSD measurements that could influence on localization behavior either as standard SSD density or assigning strain gradient for the non-local term of the model. Sampling the observed heterogeneity in dislocation density SSD or GND for 3D RVEs is considered plausible but not attempted in this work.

6. Conclusions

A proposed micromorphic enriched crystal plasticity model was used to describe RPV steel behavior at low and elevated temperatures. Micro digital image correlation measured the deformation of a miniature tensile specimen to evaluate the validity of the crystal plasticity model at the intra-grain level of polycrystalline material. The following conclusions and observations are summarized:

- Reasonable fit for the BCC crystal plasticity model was obtained in a temperature range of 123 K to 673 K in both unirradiated and irradiated conditions. This is accompanied by a critical note that the stress–strain behavior of a material is often achievable with various non-unique crystal plasticity parameter sets. However, it must be noted that since the defect structure is explicitly specified with physics-based and identifiable parameters in the present work, there is less room for such non-uniqueness. Further confidence over the model parameter choice is obtainable through the use of μ DIC experiments as well as on the selection and different variants of the modeling approach in general.
- μ DIC measurements were used to validate simulation models and assist the inherent modeling choices in terms of capturing strain localization in the material. Full-field displacements were used to define the boundary conditions for the modeling efforts. Considering the uncertainties in both experimental and computational approaches, the comparison is seen as promising and the performance of the modeling framework as satisfactory, although further areas of improvement and work were identified.

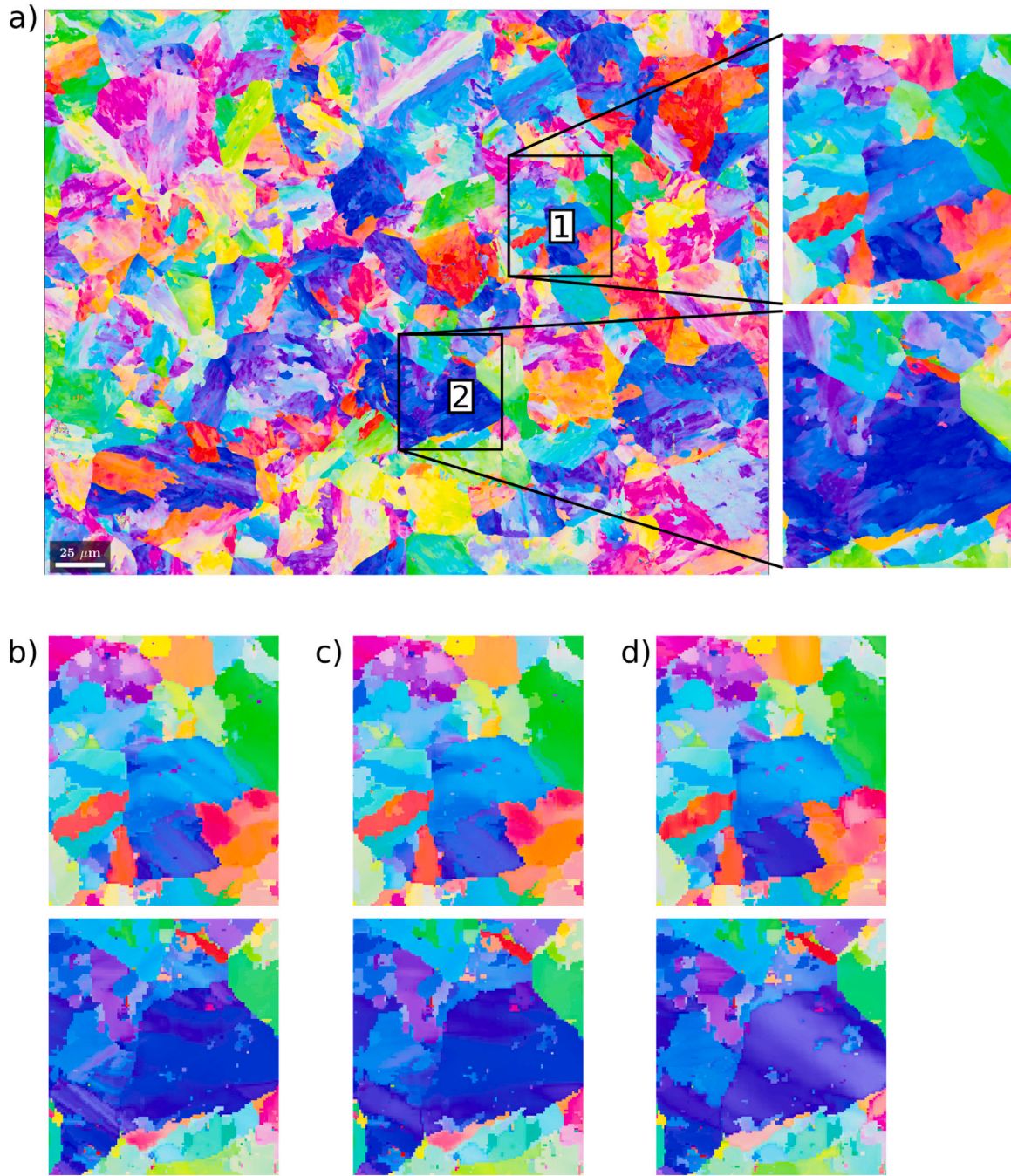


Fig. 12. IPF plot of the deformed microstructure as observed in (a) experiments (b) local CP model (c) regularized CP $H_x = 50000$, $A = 0.001$ (d) non-Schmid regularized CP $H_x = 50000$, $A = 0.001$. Two grains (labeled as 1 and 2) are compared between the experiments and the simulations. The cutout windows have a magnification of 2.2 times.

- Reduced micromorphic regularization on slip can cause over-smoothing, which can be diminished with the choice of length-scale parameters. The standard local crystal plasticity model performs reasonably well with respect to experimental data, however, it may overestimate local strains and have a general mesh dependency in the absence of non-local characteristics limiting its generalization.
- The comparison of standard Schmid's law based slip model and non-Schmid based law indicates that local deformation predictions can be improved and degraded by this choice within current

scope of work. Present work did not clearly indicate the superiority of non-Schmid behavior for the JRQ material, since the non-Schmid model provides slightly better strain magnitude prediction (not confirmed spatially), but slightly worse predictions in terms of reorientation.

- Introduction of irradiation effects promotes the plastic localization in the material at high doses and the gradient model can be used to regularize shear bands or irradiation influenced clear bands in BCC materials. At low doses, the localization effect is

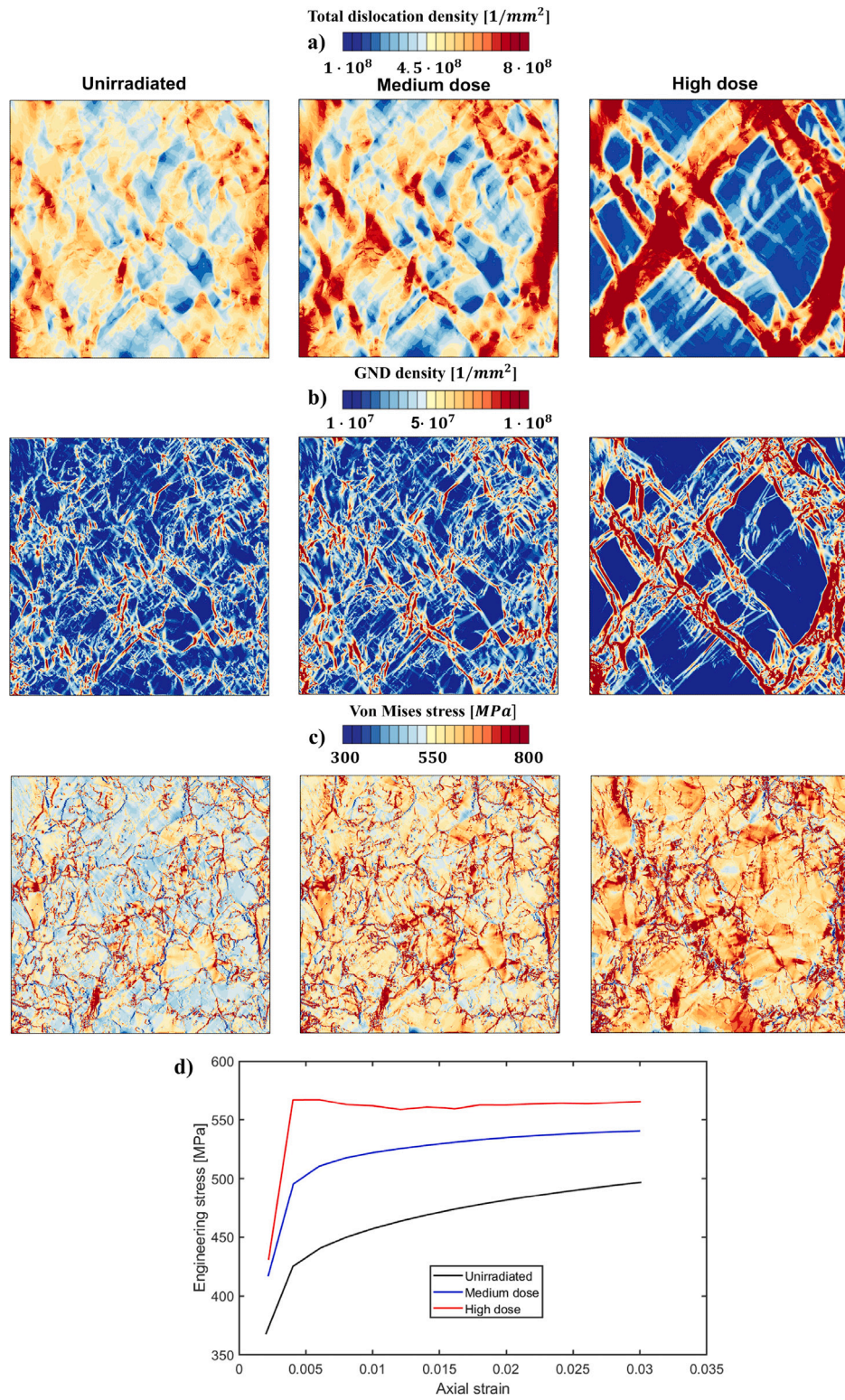


Fig. 13. (a) Total dislocation density, (b) GND density, and (c) von Mises stress of unirradiated, medium dose and high dose at the axial strain of 3%, (d) stress-strain responses of the simulated cases with the EBSD based mesh.

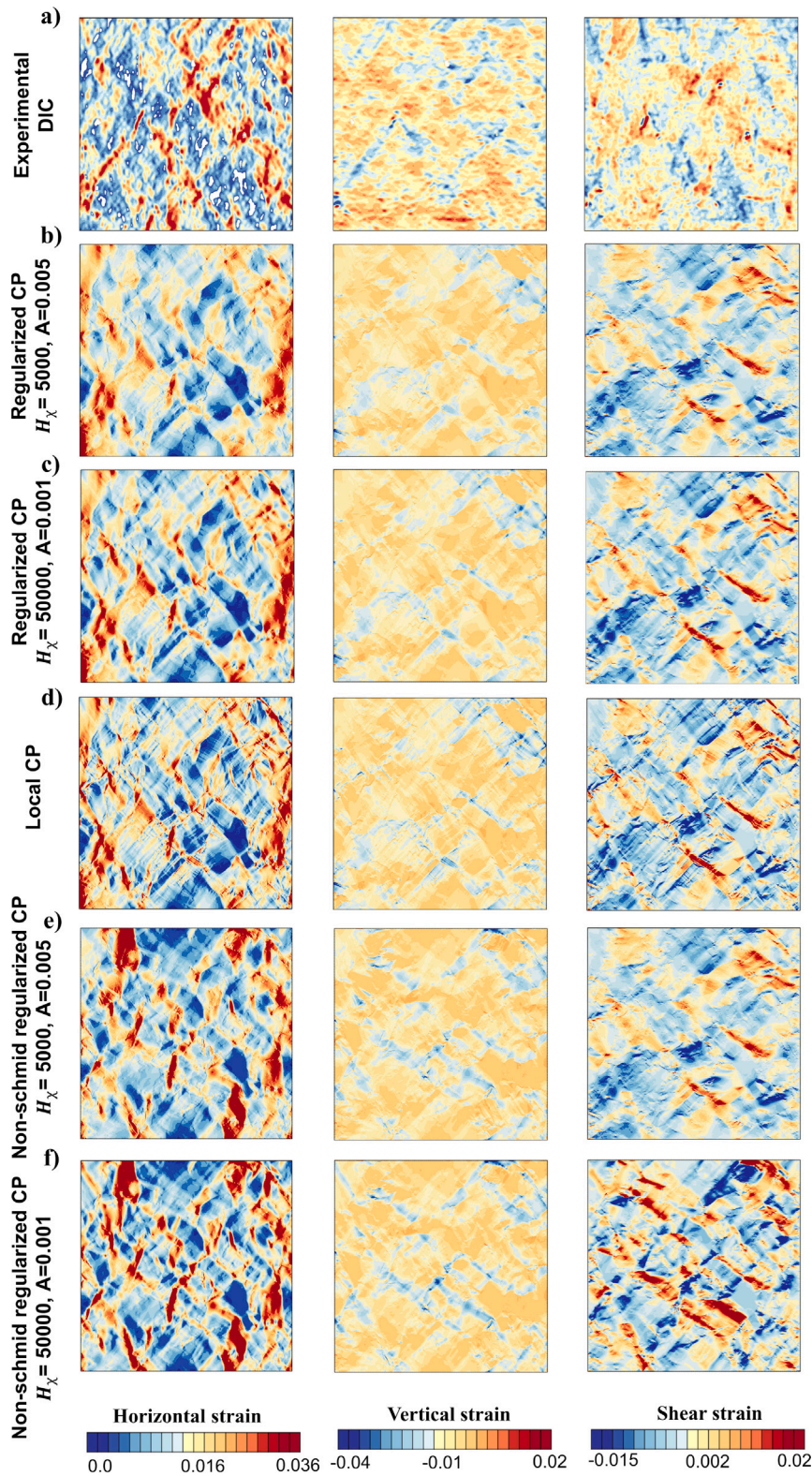


Fig. A.14. DIC experimental and simulated horizontal, vertical and shear strain fields, (a) experimental μ DIC strain fields, (b) regularized non-local plasticity with $H_x = 5000$ MPa and $A = 0.005$ N mm², (c) regularized non-local plasticity with $H_x = 50000$ MPa and $A = 0.001$ N mm², (d) local crystal plasticity, (e) Non-Schmid regularized non-local plasticity with $H_x = 5000$ MPa and $A = 0.005$, (f) Non-Schmid local plasticity with $H_x = 50000$ MPa and $A = 0.001$ N mm² at a global horizontal strain of circa 1.4%.

much more limited since the material's strain hardening capability partially suppresses localization effect in the presence of lower irradiation defect densities and their evolution (annihilation). μ DIC experiments on irradiated material samples of far higher dose should be employed in the future to validate this behavior.

An increased stress state due to irradiation affects the ductile-to-brittle transition of the material, the analyses and presented methods enable a path forward to investigate the influence of interactions arising from hardening and slip localization across a wider range of irradiation doses.

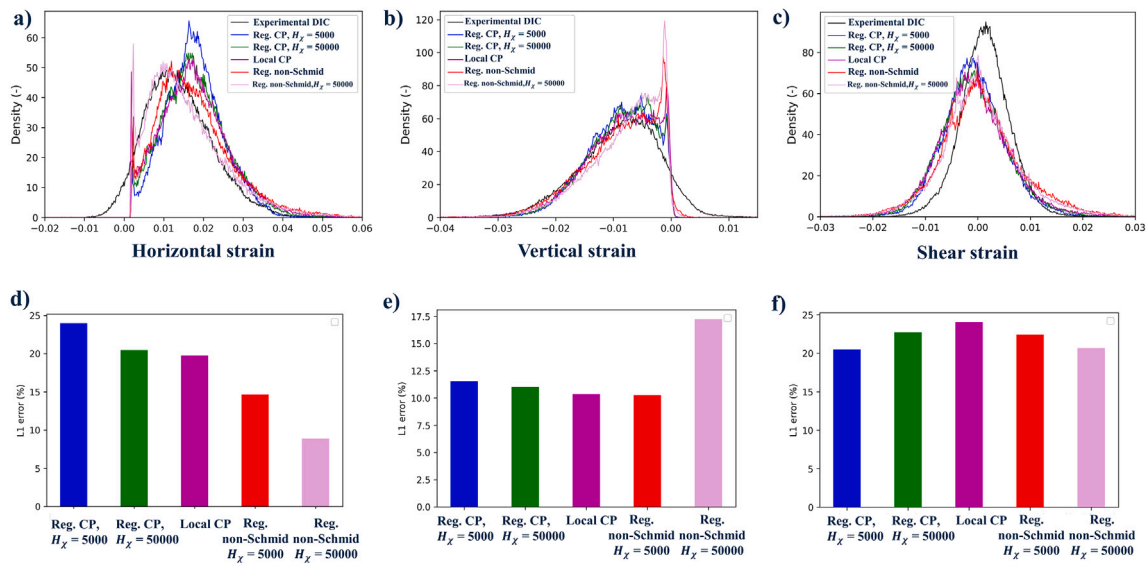


Fig. A.15. Probability density plots of (a) horizontal strain, (b) vertical strain, (c) shear strain, and the respective error bars (d)–(f), at global horizontal strain of circa 1.4%.

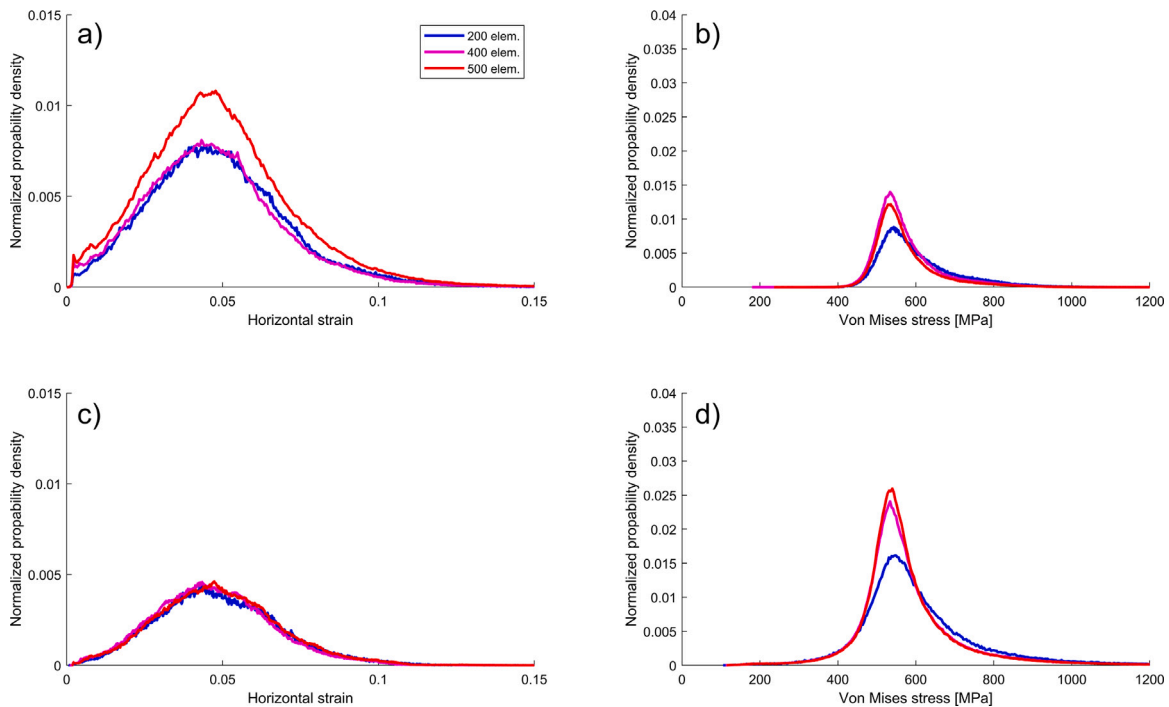


Fig. B.16. Mesh sensitivity analysis of the EBSD-DIC computational domain with horizontal strain and von Mises stress for local crystal plasticity (a) and (b), and for strain gradient approach (c) and (d) using $H_x = 50000$ MPa and $A = 0.001$ N mm² length-scale parameters.

CRedit authorship contribution statement

Matti Lindroos: Writing – original draft, Visualization, Validation, Supervision, Software, Methodology, Investigation, Data curation, Conceptualization. **Guilherme Corrêa Soares:** Writing – original draft, Visualization, Validation, Methodology, Investigation, Conceptualization. **Abhishek Biswas:** Writing – original draft, Visualization, Investigation, Conceptualization. **Wade Karlsen:** Writing – review & editing, Validation, Project administration, Data curation. **Andris Freimanis:** Writing – original draft, Software, Methodology, Conceptualization. **Sicong Ren:** Writing – review & editing, Validation, Investigation, Conceptualization. **Marta Serrano:** Project administration, Methodology, Data curation, Conceptualization. **Anssi Laukkanen:** Writing – review & editing, Software, Investigation, Conceptualization.

Declaration of competing interest

The authors declare no conflict of interest financially, personally or content-wise.

Data availability

Data will be made available on request.

Acknowledgments

This work received funding from Euratom research and training programme 2019–2020 under grant agreement No 900018 (ENTENTE

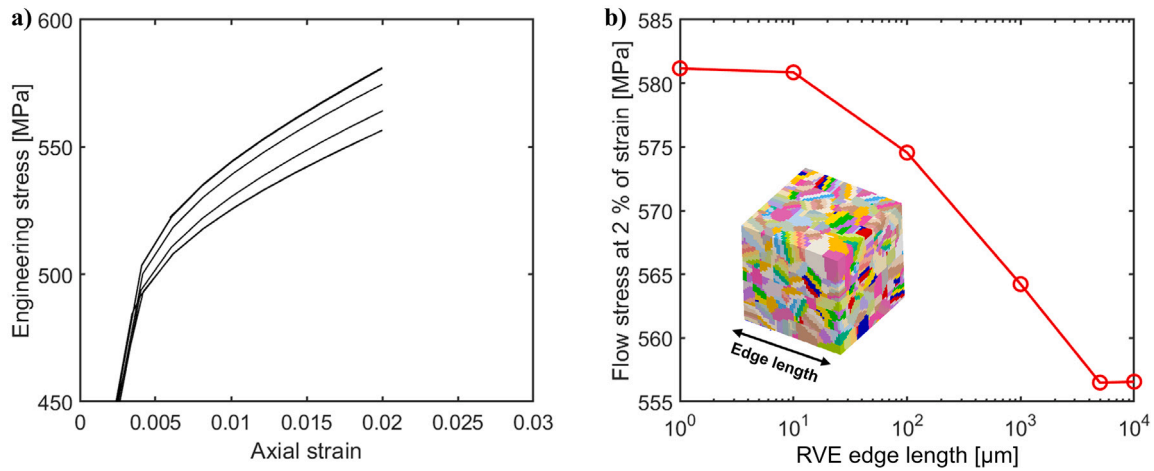


Fig. C.17. (a) Stress–strain response of different sized RVEs, (b) flow stress at 2% axial strain.

project). The authors also acknowledge the CSC – IT Center for Science, Finland, for providing computational resources. The authors acknowledge Supriya Nandy and Sneha Goel for their assistance with the EBSD characterization, Asta Nurmela for the help in in-situ testing, and Timo Veijola for their assistance with optical microscopy characterization. We thank Samuel Forest for valuable discussions related to the model framework. Nicolo Grilli is acknowledged for interesting discussions on DIC related model boundary conditions. The authors are grateful and acknowledge Miloš Kytka and Veronika Kozáková for providing one of the JRQ tensile test datasets from ÚJV Řež, a. s.

Appendix A. Low strain DIC-CP comparison

Fig. A.14 shows the comparison of horizontal, vertical and shear strains at a global axial strain of 1.4%.

Fig. A.15 shows probability density plots of different strains and error bars with respect to the experimental distribution.

Appendix B. Mesh sensitivity analysis

Fig. B.16 shows mesh sensitivity analysis for different EBSD-DIC domain discretizations for local crystal plasticity and micromorphic strain gradient model. The number of elements is indicated on the edge of the domain, for example the whole domain is 200×200 for the coarsest mesh totaling in 20 000 elements. Similarly, 500×500 discretization has a total of 250 000 elements for the same domain. It is observed that gradient model shows almost mesh insensitive solution for horizontal strain field (tensile direction). A notable difference is seen for the local crystal plasticity with the densest mesh. Both methods show some amount of mesh dependency in von Mises stress distribution. However, at higher stress values, exceeding 600 MPa, the gradient shows more or less saturated stress values when comparing 400 and 500 elements per edge discretization, while the local crystal plasticity is again more mesh sensitive.

Appendix C. Size scaling of the model

Fig. C.17 shows the stress–strain response of different sized RVEs. The scaling was applied for the whole microstructure. Original size is $100 \times 100 \mu\text{m}$. Effective grain size was kept constant at $2.5 \mu\text{m}$ to avoid scaling of the yield point and affecting dislocation density evolution with the grain size. This way, the size effects on strain hardening rate coming from the generalized stress term are observed more clearly with evolving size of the RVE. The model parameters were $H_\chi = 50000 \text{ MPa}$ and $A = 0.001 \text{ N mm}^2$ with a standard Schmid's law behavior. The model shows clear saturation of stress state at very small or large aggregate sizes.

References

- [1] A. Pineau, A. Benzerga, T. Pardoen, Failure of metals I: Brittle and ductile fracture, *Acta Mater.* 107 (2016) 424–483.
- [2] F. Beremin, A. Pineau, F. Mudry, J.-C. Devaux, Y. D'Escatha, P. Ledermann, A local criterion for cleavage fracture of a nuclear pressure vessel steel, *Metall. Mater. Trans. A* 14 (11) (1983) 2277–2287.
- [3] L. Chen, W. Liu, L. Yu, Y. Cheng, K. Ren, H. Sui, X. Yi, H. Duan, Probabilistic and constitutive models for ductile-to-brittle transition in steels: A competition between cleavage and ductile fracture, *J. Mech. Phys. Solids* 135 (2020) 103809.
- [4] A. Patra, D. McDowell, Continuum modeling of localized deformation in irradiated bcc materials, *J. Nucl. Mater.* 432 (1–3) (2013) 414–427.
- [5] T. Onchi, H. Kayano, Y. Higashiguchi, Effect of neutron irradiation on deformation behavior of zirconium, *J. Nucl. Sci. Technol.* 14 (5) (1977) 359–369.
- [6] K. Farrell, T. Byun, N. Hashimoto, Deformation mode maps for tensile deformation of neutron-irradiated structural alloys, *J. Nucl. Mater.* 335 (3) (2004) 471–486.
- [7] K. Wallin, Quantifying Tstress controlled constraint by the master curve transition temperature T_0 , *Eng. Fract. Mech.* 68 (3) (2001) 303–328, [http://dx.doi.org/10.1016/S0013-7944\(00\)00067-9](http://dx.doi.org/10.1016/S0013-7944(00)00067-9), URL: <https://www.sciencedirect.com/science/article/pii/S0013794400000679>.
- [8] K. Wallin, P. Nevasmaa, A. Laukkanen, T. Planman, Master Curve analysis of inhomogeneous ferritic steels, *Eng. Fract. Mech.* 71 (16) (2004) 2329–2346, <http://dx.doi.org/10.1016/j.engfracmech.2004.01.010>, URL: <https://www.sciencedirect.com/science/article/pii/S001379440400044X>.
- [9] P. Forget, B. Marini, L. Vincent, Application of local approach to fracture of an RPV steel: effect of the crystal plasticity on the critical carbide size, *Procedia Struct. Integr.* 2 (2016) 1660–1667, 21st European Conference on Fracture, ECF21, 20–24 June 2016, Catania, Italy.
- [10] A. Laukkanen, S. Uusikallio, M. Lindroos, T. Andersson, J. Kömi, D. Porter, Micromechanics driven design of ferritic-austenitic duplex stainless steel microstructures for improved cleavage fracture toughness, *Eng. Fract. Mech.* 253 (2021) 107878.
- [11] S. Ren, B. Marini, P. Forget, Modelling the effect of macro-segregation on the fracture toughness of heavy forgings using FFT based crystal plasticity simulations, *Eng. Fract. Mech.* 272 (2022) 108694.
- [12] F. Roters, P. Eisenlohr, L. Hantcherli, D. Tjahjanto, T. Bieler, D. Raabe, Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications, *Acta Mater.* 58 (4) (2010) 1152–1211, <http://dx.doi.org/10.1016/j.actamat.2009.10.058>, URL: <https://www.sciencedirect.com/science/article/pii/S1359645409007617>.
- [13] G. Monnet, C. Mai, Multiscale modeling of crystal plasticity in Reactor Pressure Vessel steels: Prediction of irradiation hardening, *J. Nucl. Mater.* 514 (2019) 128–138.
- [14] Z. Que, M. Lindroos, H. N., J. Lydman, P. Efsing, P. Arffman, Weld microstructure characterisation and modelling for brittle fracture initiation in a decommissioned boiling water reactor pressure vessel head, *J. Nucl. Mater.* 569 (2022) 153925.
- [15] L. Vincent, M. Libert, B. Marini, C. Rey, Towards a modelling of RPV steel brittle fracture using crystal plasticity computations on polycrystalline aggregates, *J. Nucl. Mater.* 406 (1) (2010) 91–96.
- [16] S. Bugat, J.E. Gharib, J.-M. Proix, A. Zeghadi, The toughness module of the PERFECT platform: A predictive tool for the fracture toughness of RPV steels, *J. Nucl. Mater.* 406 (1) (2010) 187–192.
- [17] A. Patra, D. McDowell, Crystal plasticity-based constitutive modelling of irradiated bcc structures, *Phil. Mag.* 92 (2012) 861–887.

- [18] N. Barton, A. Arsenlis, J. Marian, A polycrystal plasticity model of strain localization in irradiated iron, *J. Mech. Phys. Solids* 61 (2013) 341–351.
- [19] P. Chakraborty, S.B. Biner, Crystal plasticity modeling of irradiation effects on flow stress in pure-iron and iron-copper alloys, *Mech. Mater.* 101 (2016) 71–80.
- [20] P. Chakraborty, S.B. Biner, A unified cohesive zone approach to model the ductile to brittle transition of fracture toughness in reactor pressure vessel steels, *Eng. Fract. Mech.* 131 (2014) 194–209.
- [21] J. Shi, Y. Liu, Q. Xie, Z. Liu, Study on the irradiation effect of mechanical properties of RPV steels using crystal plasticity model, *Nucl. Eng. Technol.* 51 (2) (2019) 501–509.
- [22] P. Lin, J. Nie, M. Liu, Multiscale crystal plasticity finite element model for investigating the irradiation hardening and defect evolution mechanism of A508-3 steel, *Nucl. Mater. Energy* 32 (2022) 101214.
- [23] H. Ghadbeigi, C. Pinna, S. Celotto, J. Yates, Local plastic strain evolution in a high strength dual-phase steel, *Mater. Sci. Eng. A* 527 (18–19) (2010) 5026–5032.
- [24] F. Di Gioacchino, J. Quinta da Fonseca, Plastic strain mapping with sub-micron resolution using digital image correlation, *Exp. Mech.* 53 (2013) 743–754.
- [25] A. Orozco-Caballero, D. Lunt, J.D. Robson, J.Q. Da Fonseca, How magnesium accommodates local deformation incompatibility: a high-resolution digital image correlation study, *Acta Mater.* 133 (2017) 367–379.
- [26] T.E.J. Edwards, F. Di Gioacchino, A.J. Goodfellow, G. Mohanty, J. Wehrs, J. Michler, W.J. Clegg, Deformation of lamellar γ -TiAl below the general yield stress, *Acta Mater.* 163 (2019) 122–139.
- [27] S. Isavand, A. Assempour, Strain localization and deformation behavior in ferrite-pearlite steel unraveled by high-resolution in-situ testing integrated with crystal plasticity simulations, *Int. J. Mech. Sci.* 200 (2021) 106441.
- [28] D. Lunt, R. Thomas, D. Bowden, M. Rigby-Bell, S. de Moraes Shubeita, C. Andrews, T. Lapauw, J. Vleugels, J.Q. da Fonseca, K. Lambrinou, et al., Detecting irradiation-induced strain localisation on the microstructural level by means of high-resolution digital image correlation, *J. Nucl. Mater.* 580 (2023) 154410.
- [29] S. Kleinendorst, R. Fleerackers, E. Cattarinuzzi, P. Vena, D. Gastaldi, M. Van Maris, J.P. Hoefnagels, Micron-scale experimental-numerical characterization of metal-polymer interface delamination in stretchable electronics interconnects, *Int. J. Solids Struct.* 204 (2020) 52–64.
- [30] D. Lunt, A. Orozco-Caballero, R. Thomas, P. Honniball, P. Frankel, M. Preuss, J.Q. da Fonseca, Enabling high resolution strain mapping in zirconium alloys, *Mater. Charact.* 139 (2018) 355–363.
- [31] M. Lindroos, J.-M. Scherer, A. Laukkanen, T. Andersson, S. Forest, J. Vaara, A. Mantyla, T. Frondelius, Micromechanical strain gradient approach to plasticity and damage in martensitic steels, *Int. J. Plast.* 151 (2022) 103187.
- [32] M. Brumovsky, L. Davies, A. Kryukov, V. Lyssakov, R. Nanstad, Reference Manual on the IAEA JRQ Correlation Monitor Steel for Irradiation Damage Studies, Report No. IAEA-TECDOC-1230, International Atomic Energy Agency, Vienna, Austria, 2001, http://www-pub.iaea.org/MTCD/Publications/PDF/te_1230_prn.pdf.
- [33] A. Ulbricht, J. Böhmert, H.-W. Viehriig, Microstructural Analysis of the Reactor Pressure Vessel Steel A533b Cl. 1 by Small Angle Neutron Scattering, Institute of Safety Research, 2002, p. 7.
- [34] M. Brumovský, C. Faigy, T. Planman, et al., Application of surveillance programme results to reactor pressure vessel integrity assessment: Results of a coordinated research project 2000–2004, IAEA Technical Documents, International Atomic Energy Agency IAEA, Austria, 2005, number IAEA-TECDOC-1435, Project code: G5SU01067.
- [35] Z. Que, High-Temperature Water Effects on the Fracture Behaviour of Low-Alloy Reactor Pressure Vessel Steels, Technical Report, EPFL, 2019.
- [36] A.L. Medina-Almazán, L.S. Ovando-Ramírez, R. Hernández-Callejas, G. Galicia-Aguilar, Hardness and microstructural evolution of a JRQ A533 Cl. 1 steel submitted to thermal annealing, in: Pressure Vessels and Piping Conference, Vol. 51685, American Society of Mechanical Engineers, 2018, V06BT06A023.
- [37] S. Raoul, B. Marini, A. Pineau, Effect of microstructure on the susceptibility of a 533 steel to temper embrittlement, *J. Nucl. Mater.* 257 (2) (1998) 199–205.
- [38] P. Moilanen, G. Soares, M. Lindroos, A. Roiko, Design and application of a miniature pneumatic bellows loading device for in-situ tensile testing inside the scanning electron microscope, *Metals* 14 (2024) 154.
- [39] M. Zhou, G. Liu, J. Tian, H. Zhang, F. Cai, G. Xu, Microstructure and crystallography of a carbide-free bainite steel under the effect of stress, *Metall. Mater. Trans. A* 53 (6) (2022) 2226–2238.
- [40] E. Ciemat, Comportamiento frente a la irradiación neutronica de los materiales de vasijas de reactores de agua ligera, ISBN: 84-7834-186-2, 1993.
- [41] S. Preibisch, S. Saalfeld, P. Tomancak, Globally optimal stitching of tiled 3D microscopic image acquisitions, *Bioinformatics* 25 (11) (2009) 1463–1465.
- [42] J. Schindelin, I. Arganda-Carreras, E. Frise, V. Kaynig, M. Longair, T. Pietzsch, S. Preibisch, C. Rueden, S. Saalfeld, B. Schmid, et al., Fiji: an open-source platform for biological-image analysis, *Nature Methods* 9 (7) (2012) 676–682.
- [43] A. Mihal, B. Postle, C.L. Spiel, P. d'Angelo, Yuv, D. Kraft, Enblend — sourceforge.net, 2024, <https://sourceforge.net/projects/enblend/>. (Accessed 27 March 2024).
- [44] A. Mihal, C. Spiel, Combining multiple images with enblend 4.2, 2016.
- [45] P.J. Burt, E.H. Adelson, A multiresolution spline with application to image mosaics, *ACM Trans. Graph.* 2 (4) (1983) 217–236.
- [46] B. Pan, Z. Lu, H. Xie, Mean intensity gradient: an effective global parameter for quality assessment of the speckle patterns used in digital image correlation, *Opt. Lasers Eng.* 48 (4) (2010) 469–477.
- [47] A.B. Greninger, A.R. Troiano, Crystallography of austenite decomposition, *Trans. AIME* 140 (1940) 307–336.
- [48] R. Quey, M. Kasemer, The neper/fepx project: free/open-source polycrystal generation, deformation simulation, and post-processing, in: IOP Conference Series: Materials Science and Engineering, Vol. 1249, IOP Publishing, 2022, 012021.
- [49] J. Hestroffer, M. Latypov, J. Stinville, M.-A. Charpagne, V. Valle, M. Miller, T. Pollock, I. Beyerlein, Development of grain-scale slip activity and lattice rotation fields in inconel 718, *Acta Mater.* 226 (2022) 117627.
- [50] U. Kocks, A. Argon, M. Ashby, Thermodynamics and kinetics of slip, *Progress in Materials Science*, Pergamon Press, 1975, URL: <https://books.google.fi/books?id=BOAkMgEACAAJ>.
- [51] N. Castin, G. Bonny, M. Konstantinovic, A. Bakaev, F. Bergner, C. Courilleau, C. Domain, B. Gomez-Ferrer, J. Hyde, L. Messina, G. Monnet, M. Pascuet, B. Radiguet, M. Serrano, L. Malerba, Multiscale modelling in nuclear ferritic steels: From nano-sized defects to embrittlement, *Mater. Today Phys.* 27 (2022) 100802.
- [52] P.-D. Lin, J.-F. Nie, Y.-P. Lu, C.-X. Shi, S.-G. Cui, Atomic irradiation defects induced hardening model in irradiated tungsten based on molecular dynamics and CPFEM, *Int. J. Plast.* 174 (2024) 103895.
- [53] S. Lee, H. Cho, C. Bronkhorst, R. Poharel, D. Brown, B. Clausen, S. Vogel, V. Anghel, G.G. III, J. Mayeur, Deformation, dislocation evolution and the non-schmid effect in body-centered-cubic single- and polycrystal tantalum, *Int. J. Plast.* 163 (2023) 103529.
- [54] K. Ammar, S. Forest, H. Kahla, D. Mereib, M. Laurent-Brocq, Unravelling the extra-hardening in chemically architected high entropy alloys, *Comput. Mater. Sci.* 233 (2024) 112714.
- [55] R. Gröger, A. Bailey, V. Vitek, Multiscale modeling of plastic deformation of molybdenum and tungsten: I. Atomistic studies of the core structure and glide of 1/2(111) screw dislocations at 0 K, *Acta Mater.* 56 (19) (2008) 5401–5411.
- [56] M. Lindroos, N. Vajragupta, J. Heikinheimo, D. Ribeiro-Costa, A. Biswas, T. Andersson, P. Olsson, Micromechanical modeling of single and polycrystalline UO_2 at elevated temperatures, *J. Nucl. Mater.* 573 (2023) 154127.
- [57] M. Lindroos, T. Pinomaa, K. Ammar, A. Laukkanen, S. Forest, N. Provatas, Dislocation density in cellular rapid solidification using phase field modeling and crystal plasticity, *Int. J. Plast.* 148 (2022) 103139.
- [58] R. Chaouadi, R. Gerard, E. Stergar, W.V. Renterghem, Neutron irradiation hardening of chemically-tailored RPV steels with respect to Cu/P and Ni/Mn elements, *J. Nucl. Mater.* 519 (2019) 188–204.
- [59] E. Altstadt, A. Ballesteros, F. Bergner, I. O'Donnell, P. Efsing, H. Hein, M. Malerba, S. Ortner, T. Planman, RPV irradiation embrittlement: NUGENIA position on RPV irradiation embrittlement issues based on the outcome of the EURATOM FP7 project LONGLIFE, *Nugenia* (2015) 1–27.
- [60] C. Dethloff, E. Gaganidze, J. Aktaa, Review and critical assessment of dislocation loop analyses on EUROFER 97, *Nucl. Mater. Energy* 15 (2018) 23–26.
- [61] B. Gómez-Ferrer, C. Dethloff, E. Gaganidze, L. Malerba, C. Hatzoglou, C. Pareige, Nano-hardening features in high-dose neutron irradiated Eurofer97 revealed by atom-probe tomography, *J. Nucl. Mater.* 537 (2020) 152228.
- [62] C. Cabet, F. Dalle, E. Gaganidze, J. Henry, H. Tanigawa, Ferritic-martensitic steels for fission and fusion applications, *J. Nucl. Mater.* 523 (2019) 510–537.
- [63] M. Klimenkov, U. Jäntschi, M. Rieth, A. Möslang, Correlation of microstructural and mechanical properties of neutron irradiated EUROFER97 steel, *J. Nucl. Mater.* 538 (2020) 152231.
- [64] M. Abatour, S. Forest, Strain gradient plasticity based on saturating variables, *Eur. J. Mech. A Solids* (2023) 105016.
- [65] M. Borde, L. Dupuy, A. Pivano, B. Michel, D. Rodney, J. Amodeo, Interaction between 1/2 110001 dislocations and 110 prismatic loops in uranium dioxide: Implications for strain-hardening under irradiation, *Int. J. Plast.* 168 (2023) 103702.
- [66] A. Li, W. Hu, Y. Yang, K. Li, H. Tian, Z. Zhan, Q. Meng, A microdamage model for FCC single crystals considering a mixed failure mechanism of slip and cleavage, *Int. J. Plast.* 173 (2024) 103888.
- [67] M. Salvini, N. Grilli, E. Demir, S. He, T. Martin, P. Flewitt, M. Mostafavi, C. Truman, D. Knowles, Effect of grain boundary misorientation and carbide precipitation on damage initiation: A coupled crystal plasticity and phase field damage study, *Int. J. Plast.* 172 (2024) 103854.
- [68] W. Wen, L. Capolungo, A. Patra, C. Tome, A physics-based crystallographic modeling framework for describing the thermal creep behavior of Fe-Cr alloys, *Metall. Mater. Trans. A* 48 (2017) 2603–2617.
- [69] G. Po, Y. Huang, Y. Li, K. Baker, F. Flores, T. Black, J. Hollenbeck, N. Ghoniem, A model of thermal creep and annealing in finite domains based on coupled dislocation climb and vacancy diffusion, *J. Mech. Phys. Solids* 169 (2022) 105066.