Crystal plasticity finite element analysis of nanoindentation process in Eurofer97 at elevated temperatures

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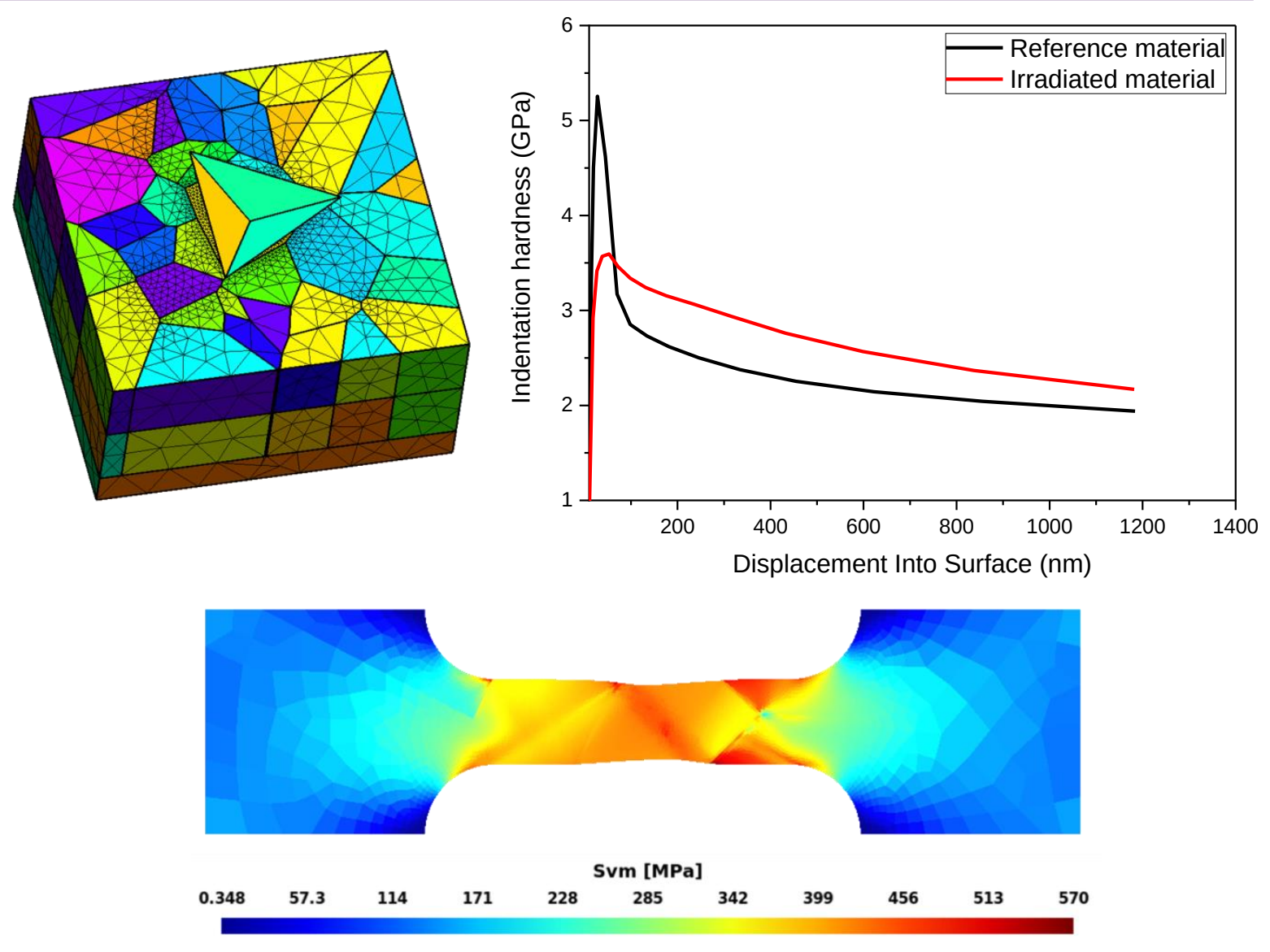
Introduction

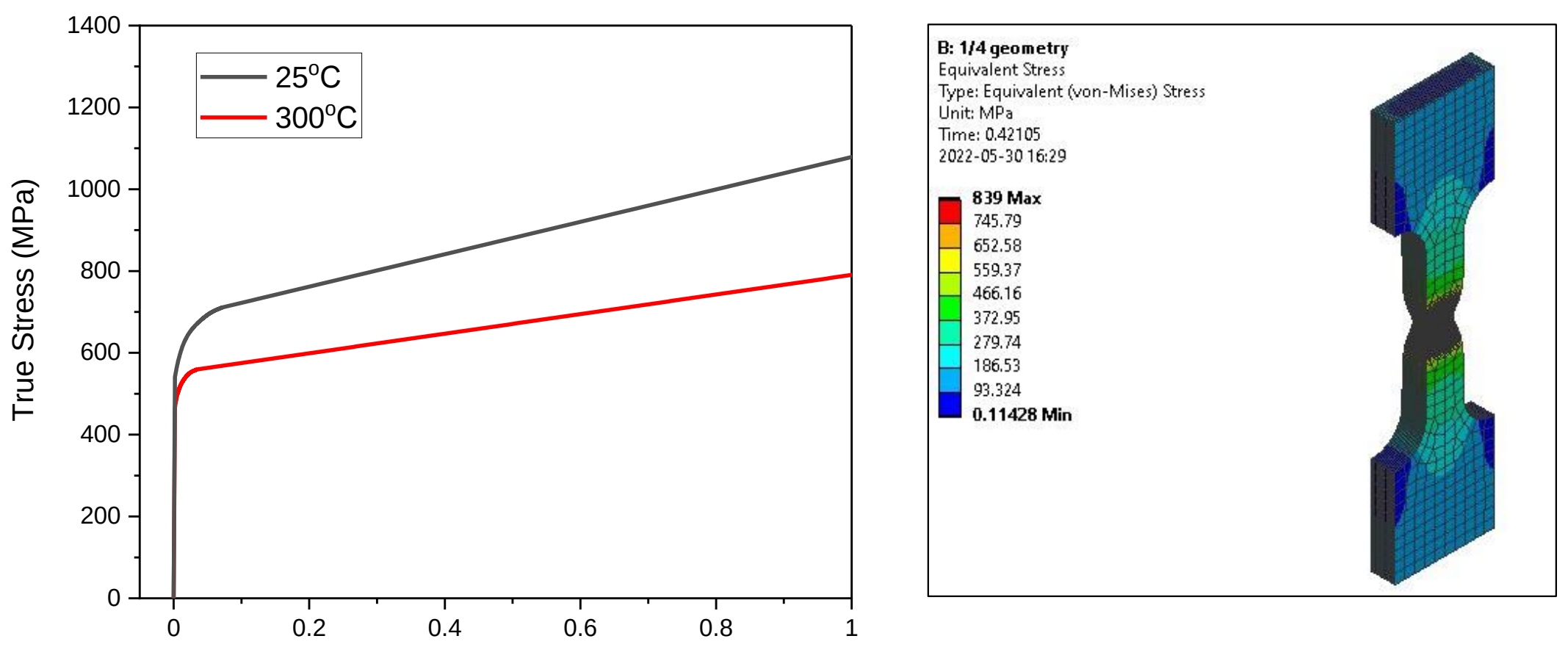
The application of nanoindentation in nuclear materials science rapidly emerges because it is non-destructive method allowing to deduce important mechanical characteristics, while using extremely small volume of probing material. The probing range of hundreds nanometers to several micrometers, enables the characterization of damage done by heavy ion irradiation which can be applied to surrogate the neutron damage. In this work we use the crystal plasticity finite element method (CPFEM) to simulate the nanoindentation process on Eurofer97 RAFM steel in a range of temperatures. The constitutive parameters describing the elastoplastic behavior of the material are obtained from the conventional tensile tests or literature. This work is being an *initial step* of the model development, and serves as a basis for further implementation of the ion-induced non-uniform damage layer and its' impact on the mechanical properties.

Objectives

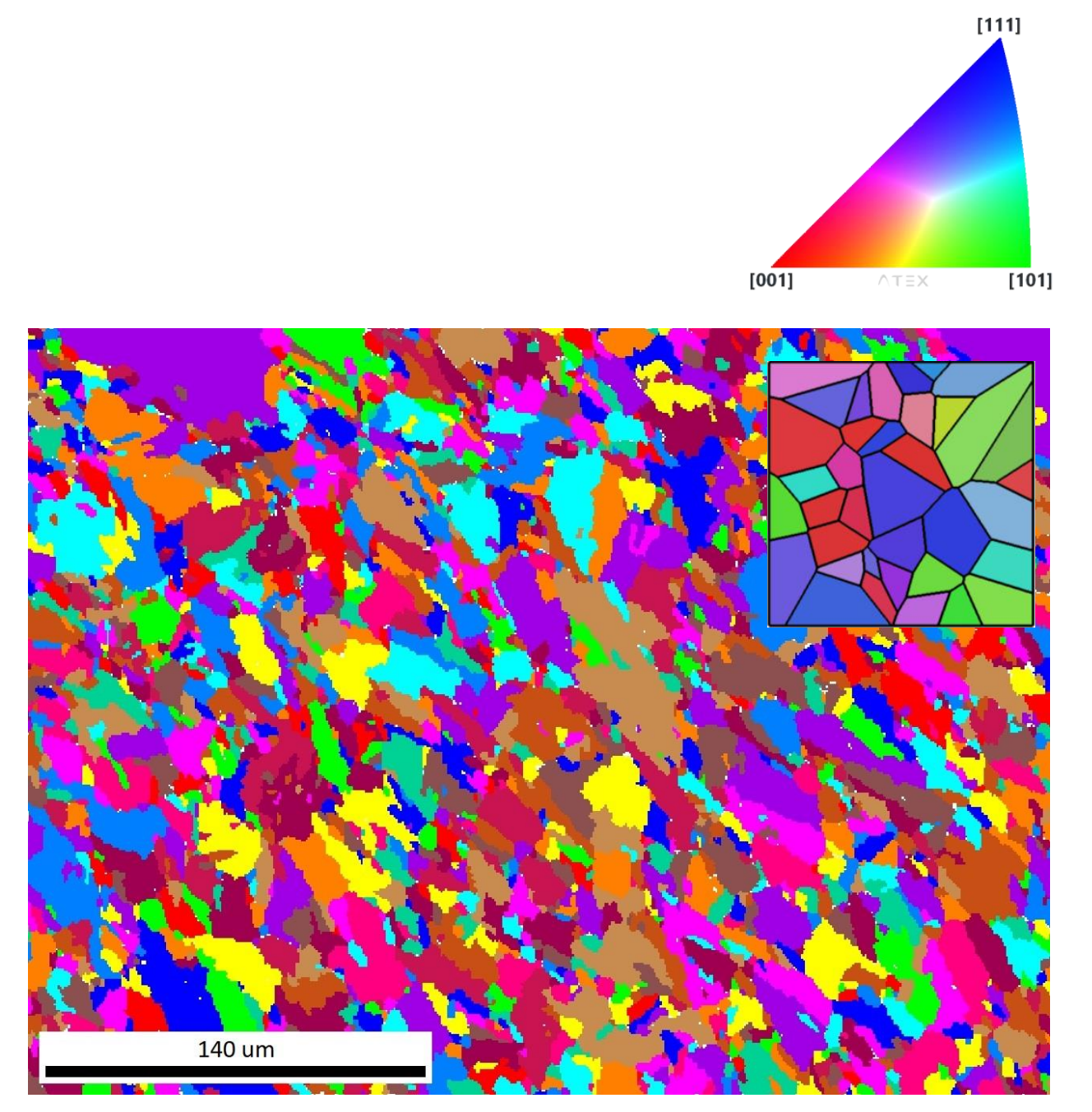
- Development and validation of FEM nanoindentation model in a range of temperatures
- Implementation of the irradiation effect for the extraction of constitutive laws of ion-irradiated material, i.e. assessment of the irradiation hardening on constitutive laws
- Simulations of conventional tests using constitutive parameters for irradiated material obtained with FEM nanoindentation model



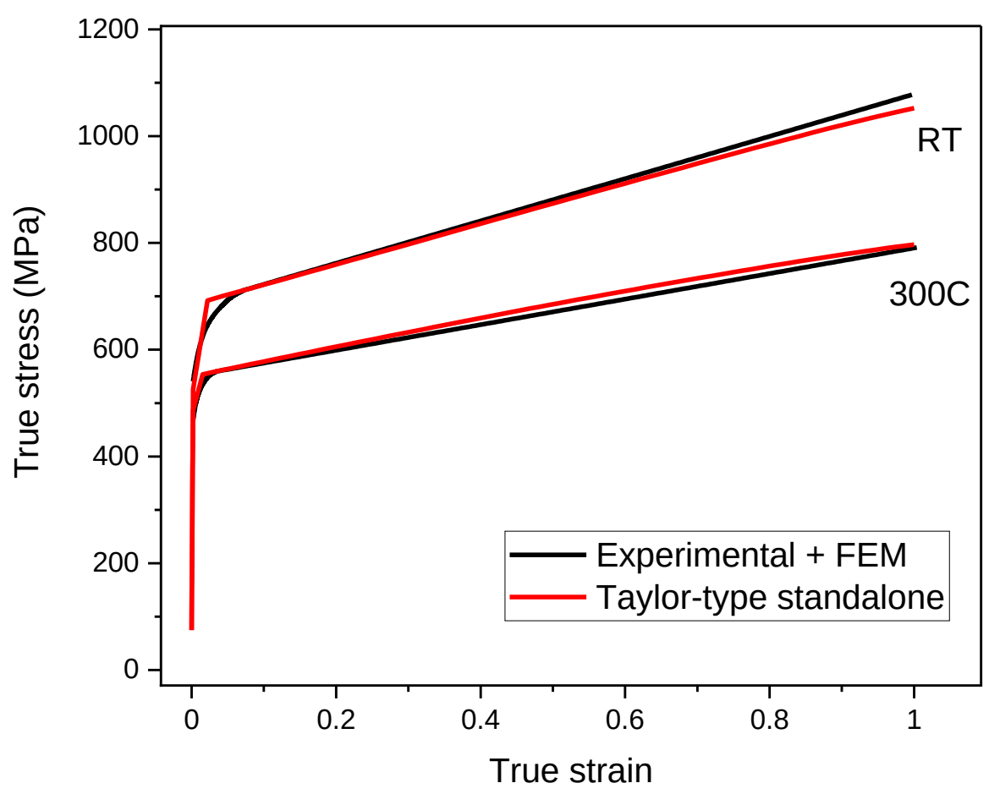
Methods



1. Experimental stress-strain curve with the corrected elastic part recalculated into true stress-strain until UTS; The curve is predicted from UTS to 100% of strain by using dogbone simulations

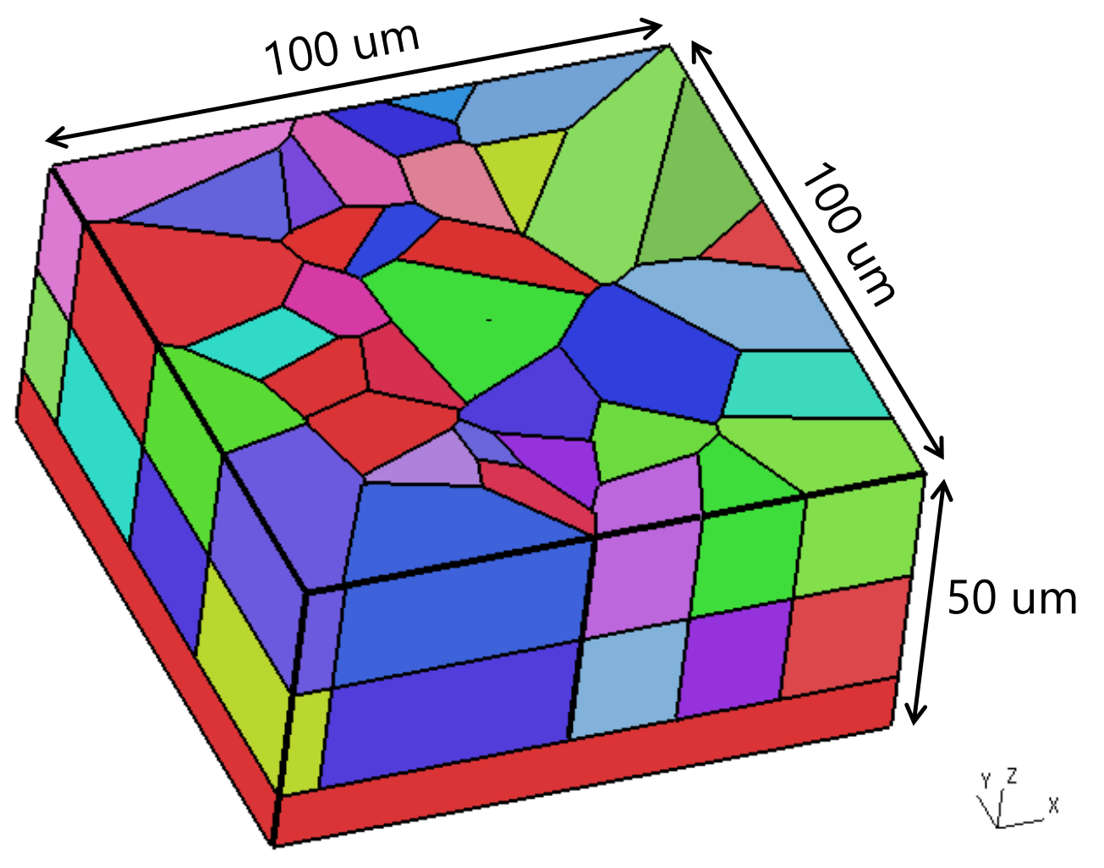


EBSD map of E97 steel (15° misorientation) in comparison with FEM polycrystal model surface



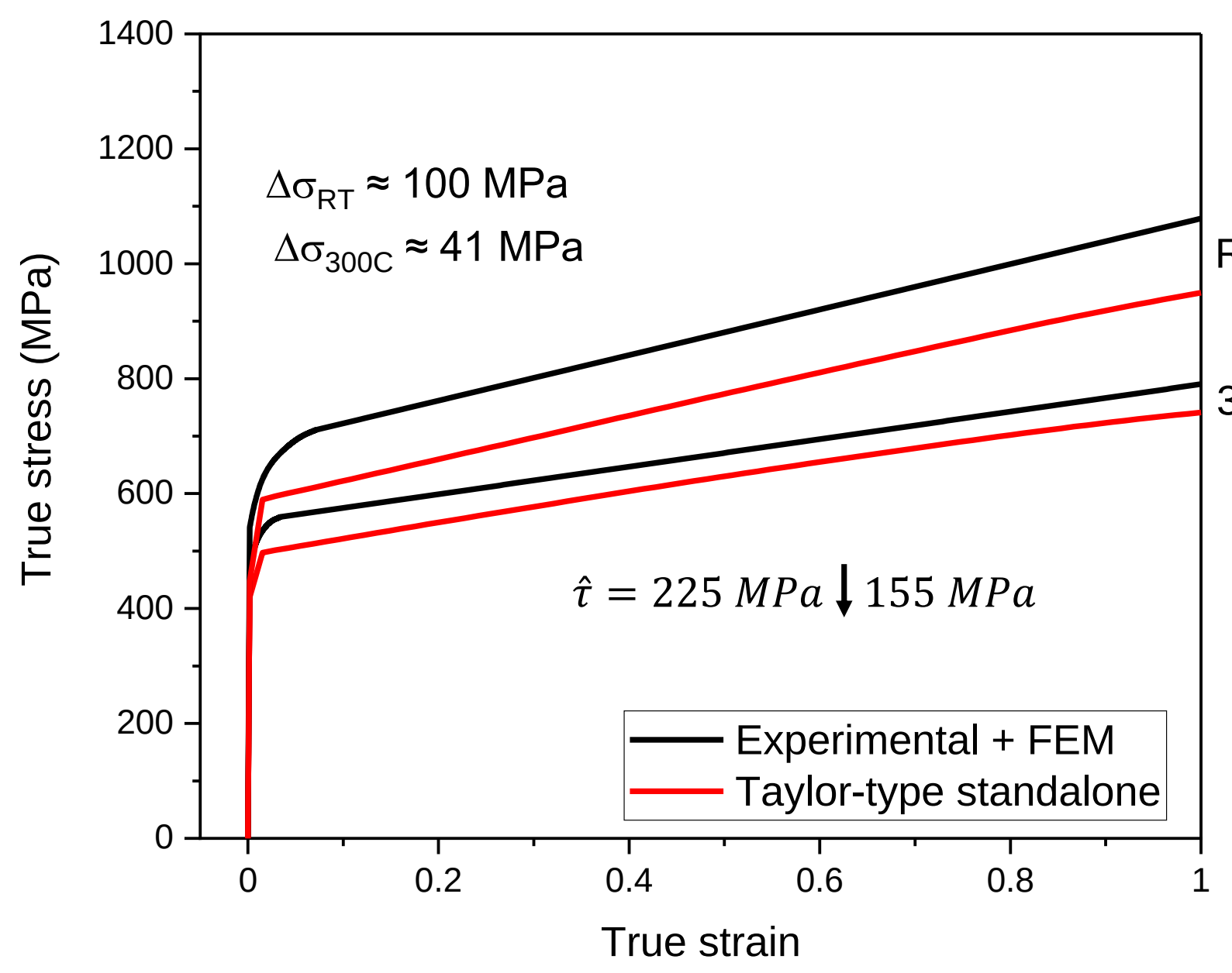
Parameter	Value	Source
Elastic coefficient, *C11*	230 *GPa*	Literature
Elastic coefficient, *C12*	135 *GPa*	Literature
Elastic coefficient, *C44*	117 *GPa*	Literature
Reference slip rate, $\dot{\gamma}_0$	10^5 s^{-1}	Fitted
Activation energy, $2H_k$	2.365 *eV*	Literature/ Artificially increased
Hall-Petch + Lattice friction, S_0	78.0 *MPa*	Fitted
Burger's vector, *b*	0.2482 *nm*	Literature
Initial dislocation density, ρ_0	$1.5 \cdot 10^{14}$ m^{-2}	Measured
Dislocations interaction coefficient, h_{dis}	0.32	Fitted
Saturated dislocation density, ρ_{sat}	$3.45 \cdot 10^{16}$	Fitted
Kocks-Mecking parameter, k_1	$1.55 \cdot 10^7$ m^{-1}	Fitted
Pierels barrier constant, *p*	0.5	Literature
Pierels barrier constant, *q*	1.5	Literature
Thermal stress, $\hat{\tau}$	225.0 MPa	Fitted

2. The constitutive parameters are established using different sources; The true stress-strain curves for different temperatures are replicated with a simulation of uniaxial tension of 1000 randomly oriented grains

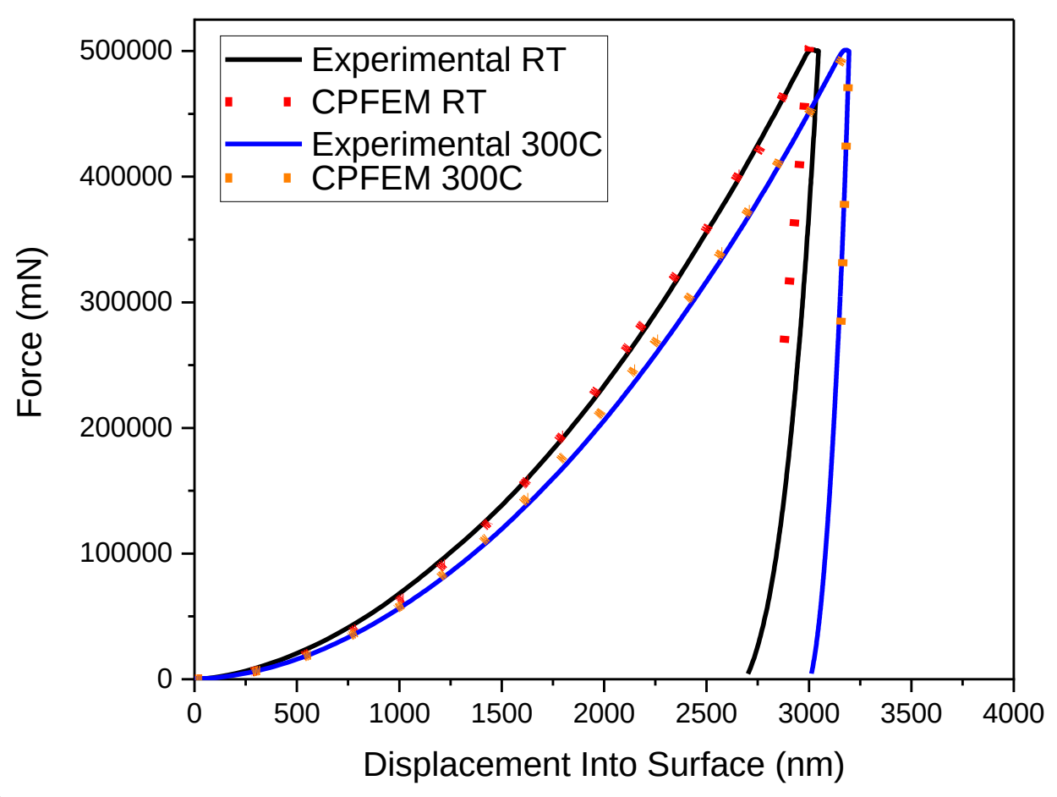


3. The obtained constitutive laws are used as an input for CPFEM model of Berkovich indenter immersion into 17 µm grain size randomly oriented polycrystal

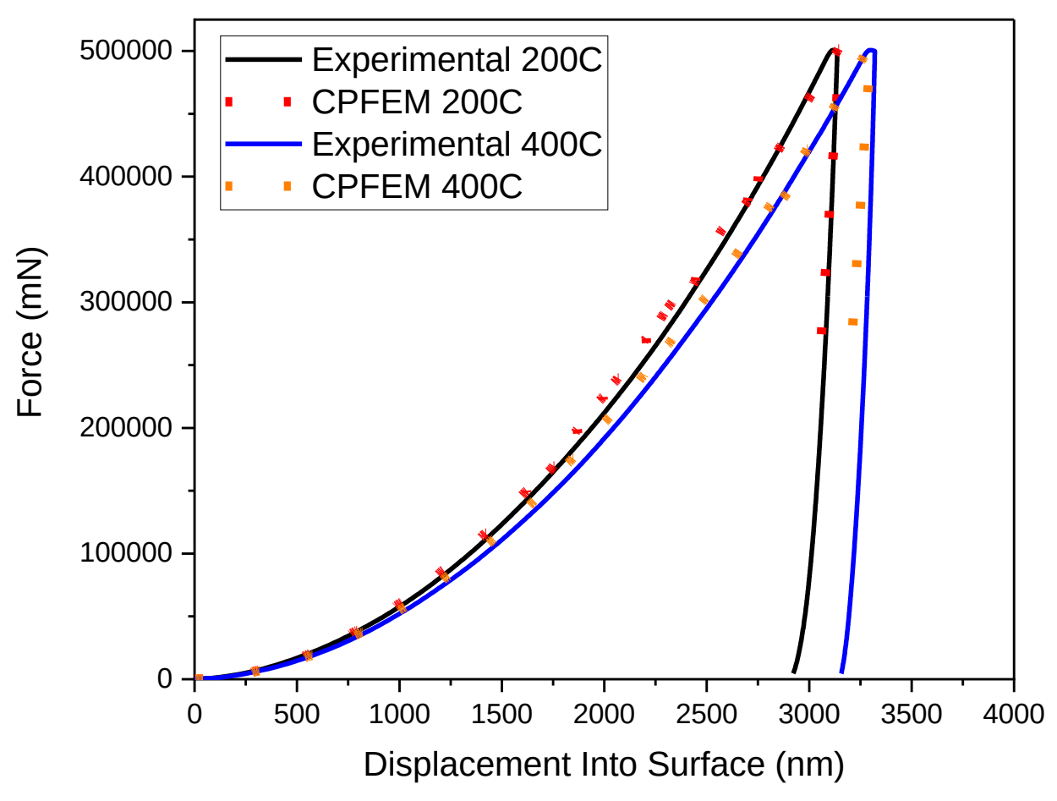
Results



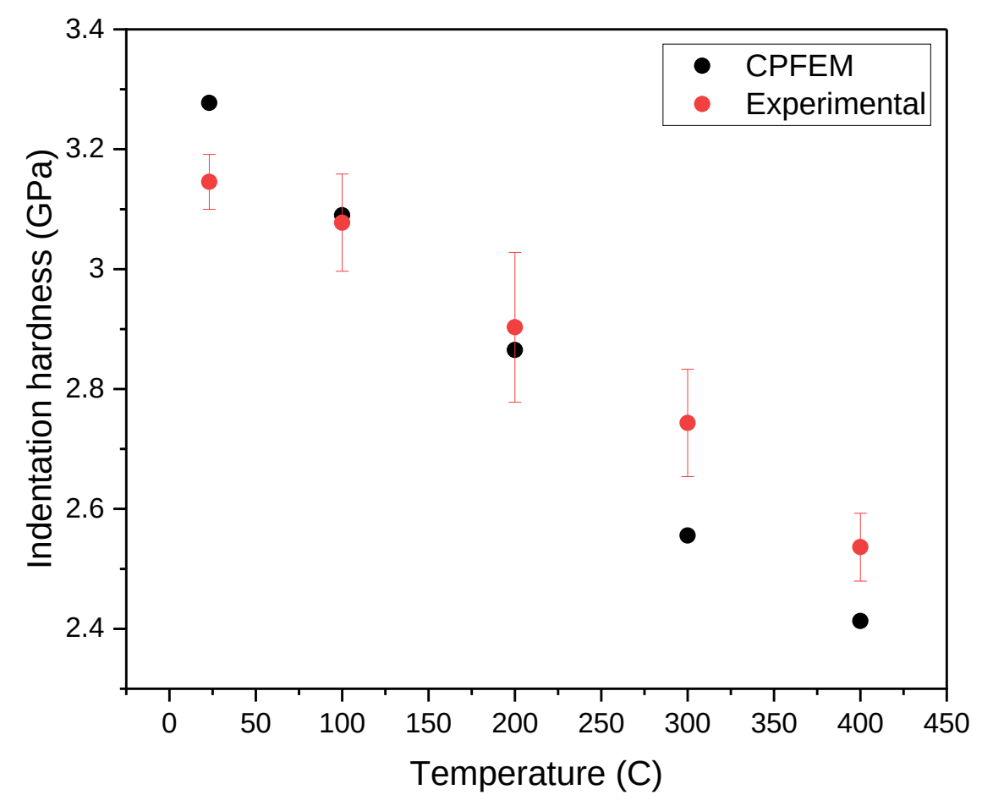
The grain boundaries stress contribution from large prior austenite grains (30 – 50 µm) is not significant enough for nanoindentation, but it is for tensile testing. Therefore, the thermal stress parameter has been lowered in order to exclude it from nanoindentation simulations.



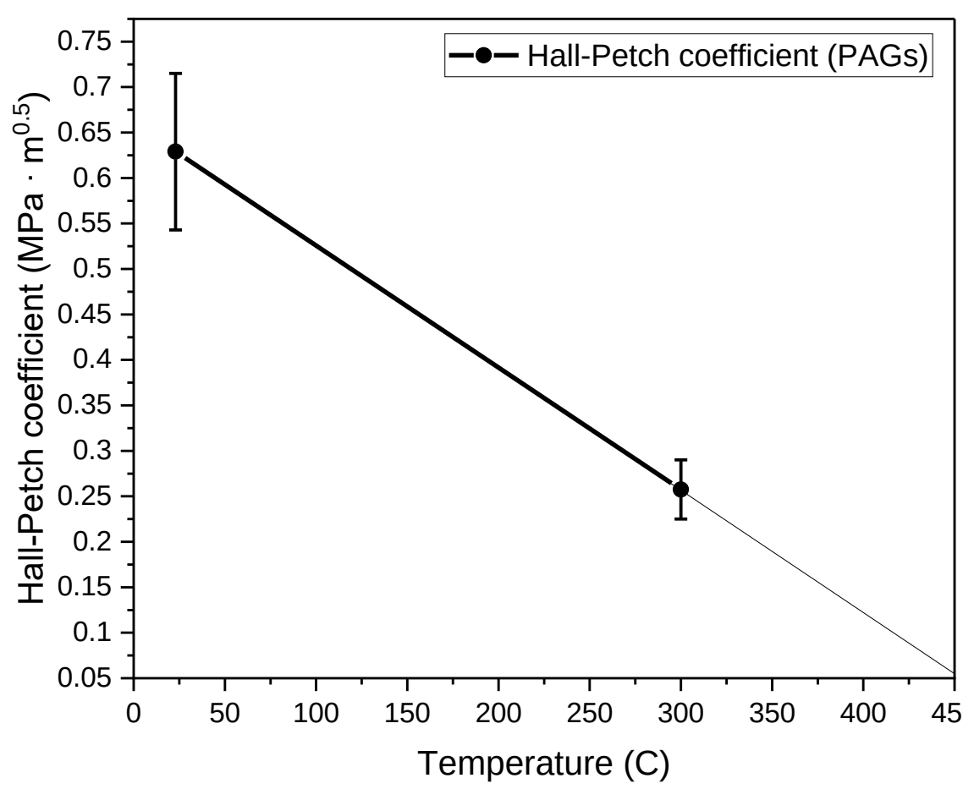
Simulated and experimental nanoindentation force-displacement curves for room temperature and 300°C



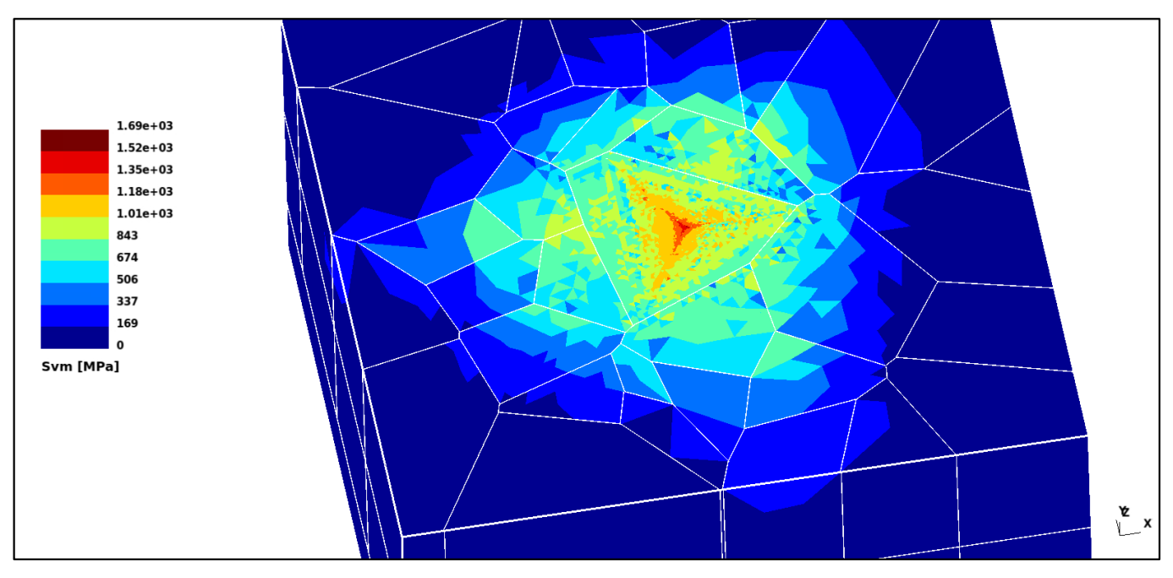
Simulated and experimental nanoindentation force-displacement curves for 200°C and 400°C



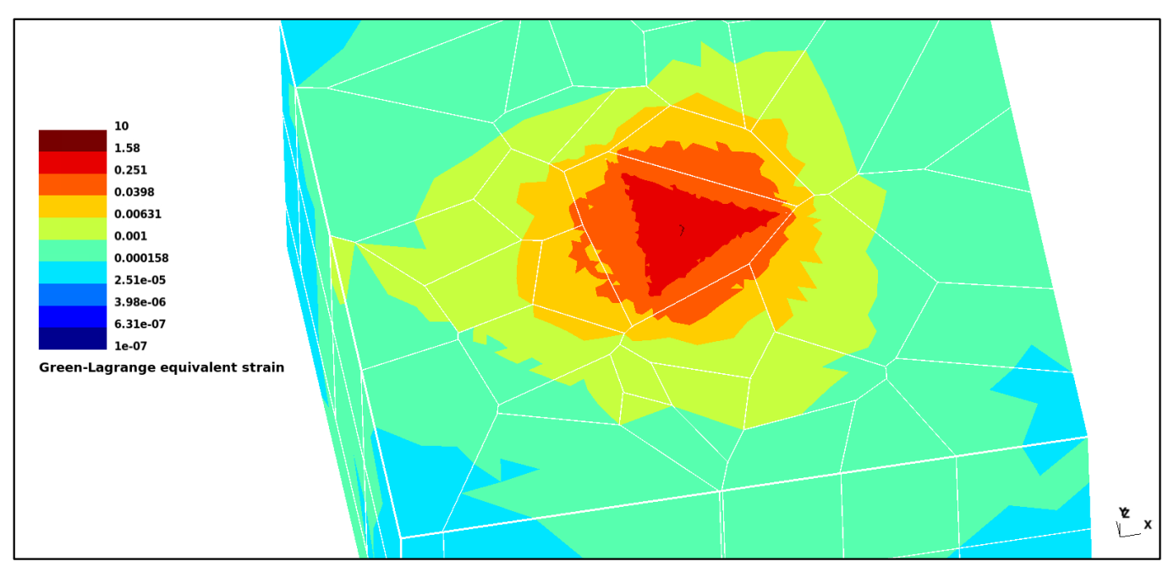
Indentation hardness vs. temperature calculated experimentally and from simulations



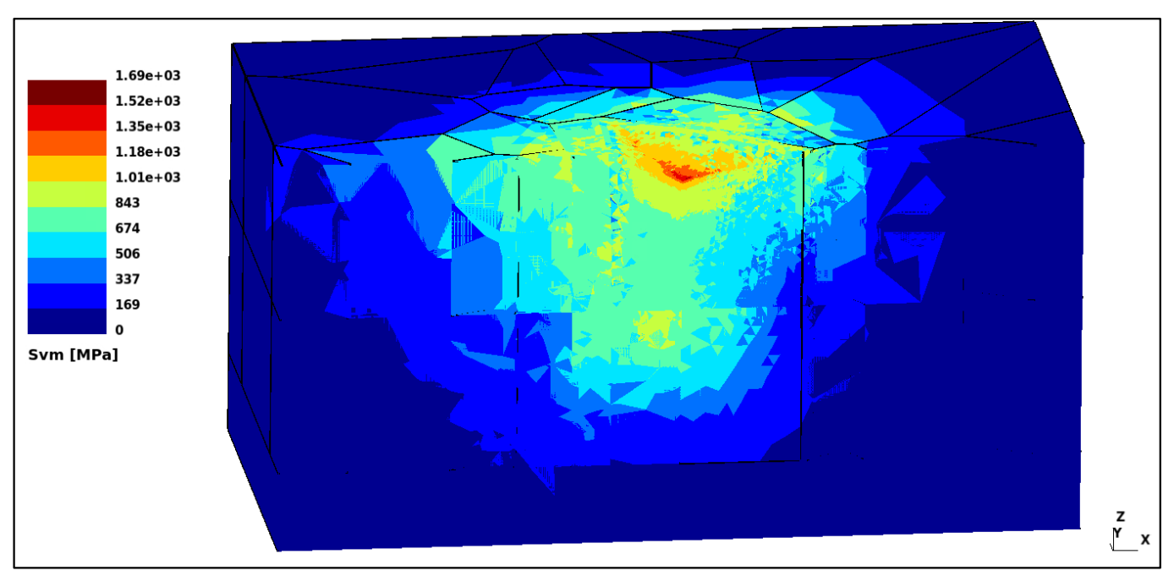
Hall-Petch coefficient for prior austenite grains in E97 calculated based on the differences of yield stress



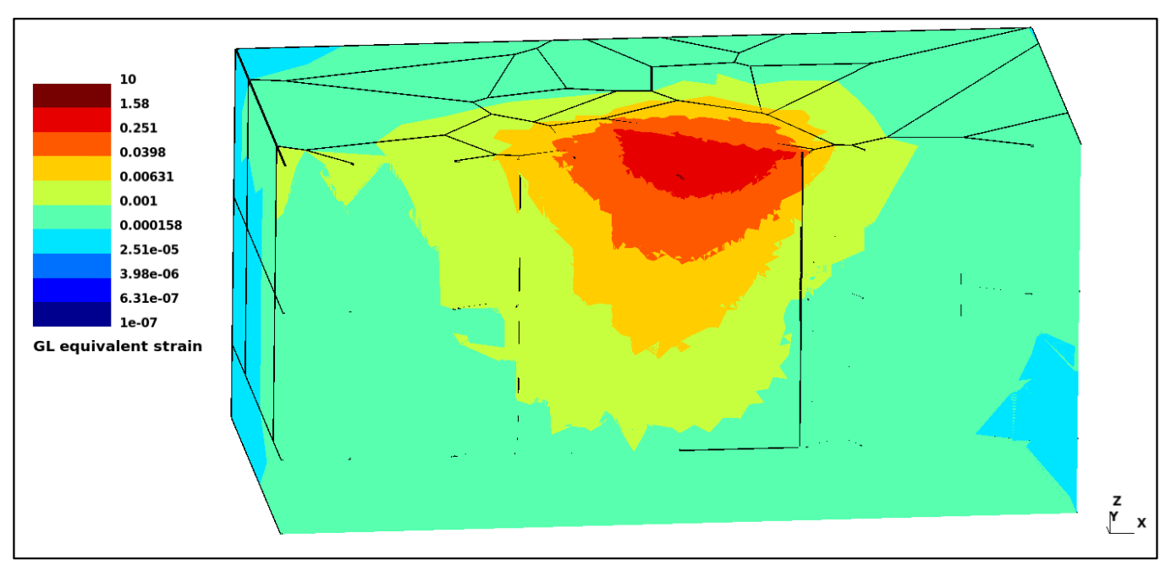
Von Mises stress distribution on the indented surface



Equivalent strain distribution on the indented surface



Von Mises stress distribution along the indentation direction



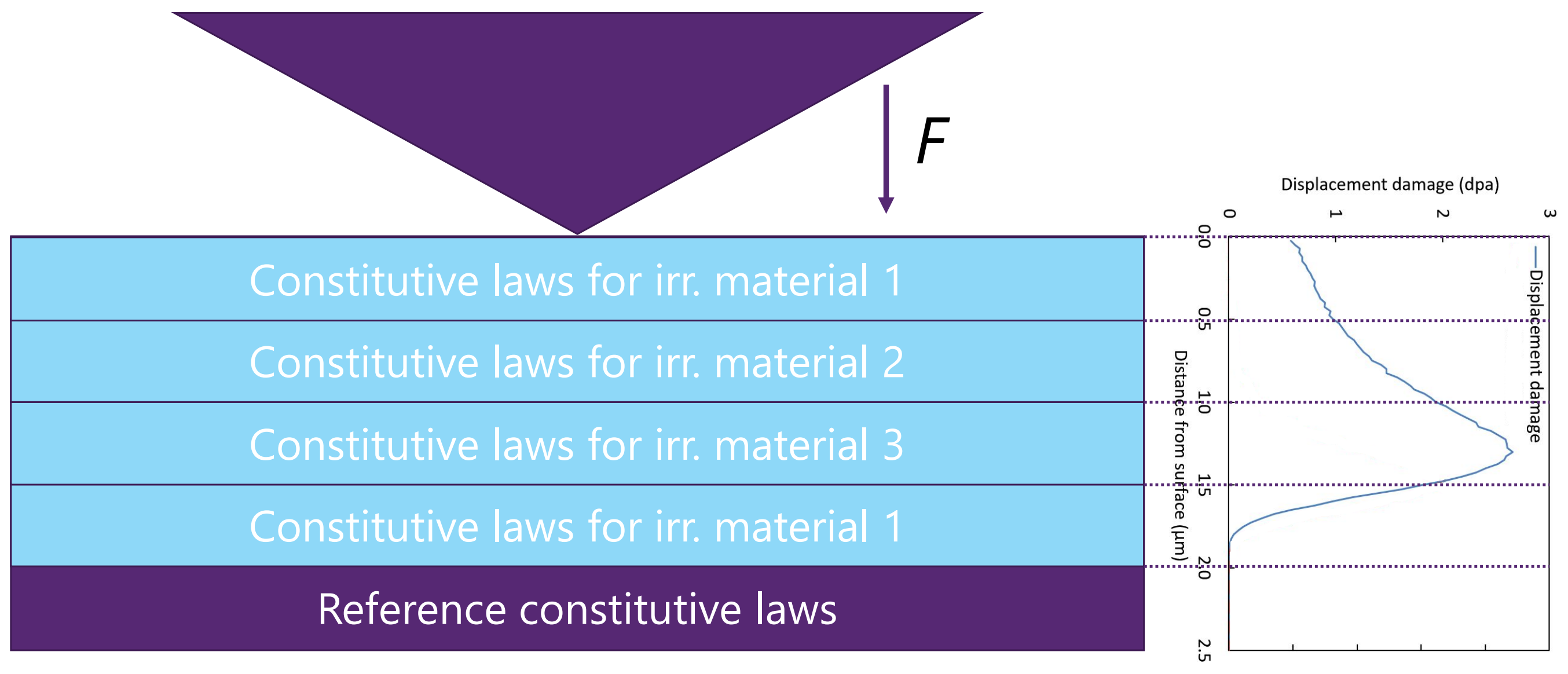
Equivalent strain distribution along the indentation direction

Discussion

This work is the first step towards the development of the CPFEM model which could treat the heterogeneous microstructure generated by the ion irradiation damage and thereby help to retrieve the local property of the material. It is expected that the magnitude of the irradiation hardening can be associated with the damage dose and potentially linked to the damage caused by neutrons. See figure below.

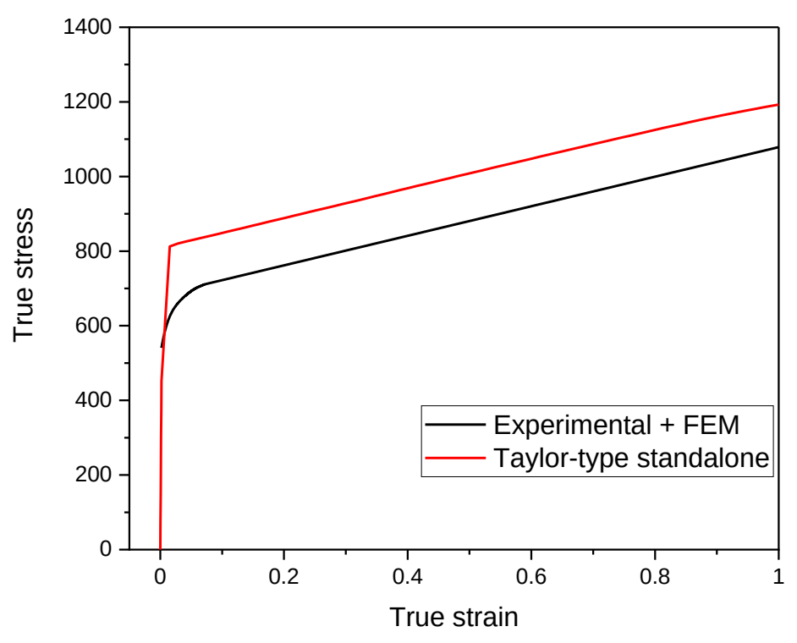
The presented computational approach is a prospective tool to investigate the mechanical response of the material to the compressive deformation under nanoindentation experimental conditions. On the one hand, the approach adequately grasps the heterogeneity of the plastic deformation under indenter, and on the other hand it correctly transfers the constitutive law derived from the tensile tests.

The computational approach remains rather flexible to introduce other mechanisms standing for the mechanical properties degradation due to the irradiation, such as creep models or Gurson models (irradiation swelling), with the consequent validation and analysis. The model could be useful for characterization of a material exhibiting the irradiation strain softening, and with an implementation of the strain gradient theory could be able to help to distinct the indentation size effect from irradiation hardening.

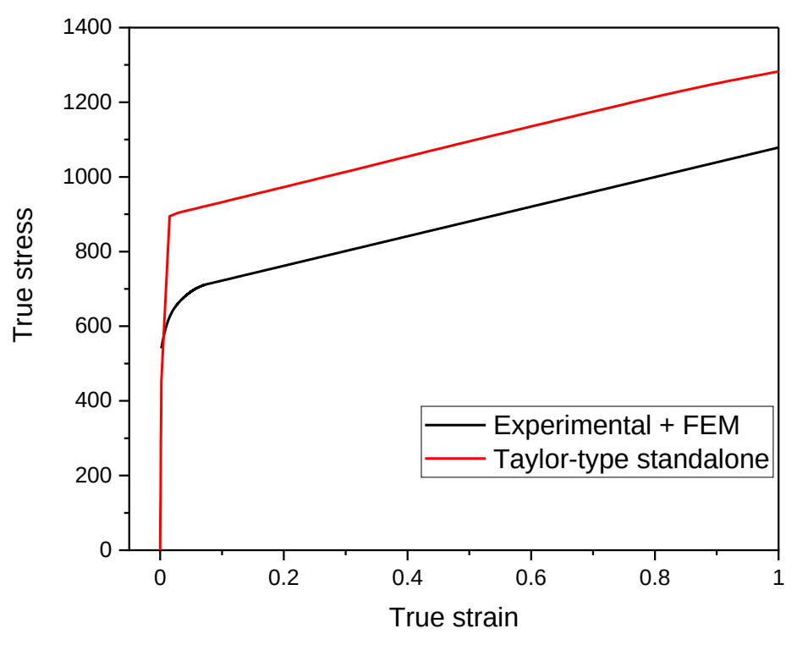


Constitutive laws for irr. material 1
Constitutive laws for irr. material 2
Constitutive laws for irr. material 3
Constitutive laws for irr. material 1
Reference constitutive laws

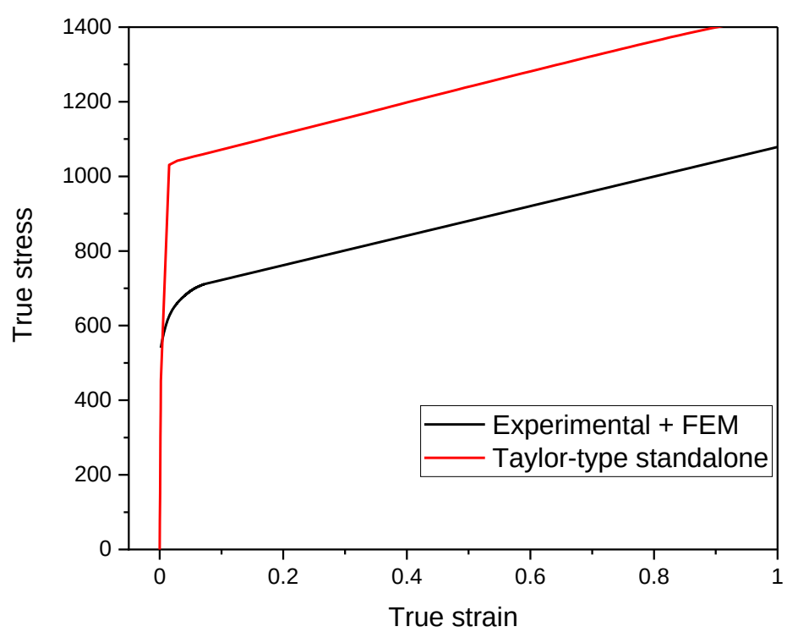
The possible implementation of the ion irradiation damage. The sub-surface is split into layers, where each layer, with dedicated constitutive laws corresponds to a particular magnitude of displacement damage. The constitutive laws (yield stress) for the each layer are modified until the good match with validation experiments is obtained.



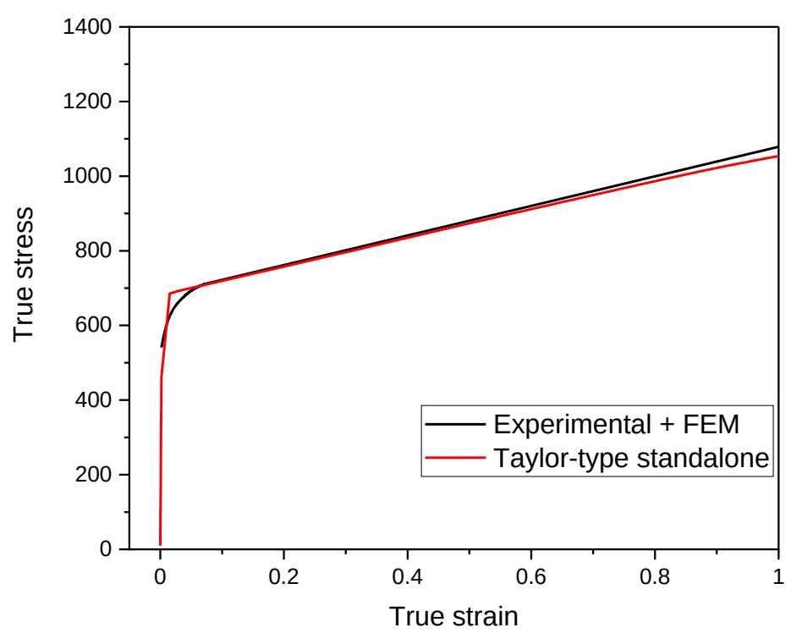
Constitutive laws for irr. material 1



Constitutive laws for irr. material 2



Constitutive laws for irr. material 3



Reference constitutive laws

Conclusions

- The set of the constitutive parameters defined from the tensile experiments is precise enough to reproduce true stress-strain curves of the studied material and in combination with presented CPFEM nanoindentation setup can also reproduce the nanoindentation F-d curves of the same material and testing conditions.
- Not only the outcoming F-d curves, but also hardness values were replicated quite well from the simulation and by using the Oliver-Pharr method for the perfect indenter, which is our case in this approach.
- The presented approach can be also used for studying the grain boundary effects, and depending on the indentation depth it appears to be possible to choose the microstructural feature to study, if their dimensions are different enough.
- The mathematical functional and CPFEM model are perfectly suitable for the incorporation of the non-uniformly distributed irradiation defects (such as dislocation loops and voids) given that the thermally-activated dislocation-defect interaction can be parameterized based on the available theoretical and atomistic modelling studies.

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