Constitutive description and FEM implementation of 316L stainless steel material model

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Abstract
In the present work, a constitutive model materials undergoing the plastic strain induced phase transformation has been developed. The model is based on the linearized transformation kinetics, which is relevant for the cryogenic conditions. The constitutive model has been implemented in the finite element software Abaqus/Explicit by means of the external user subroutine VUMAT, which incorporates the user defined plasticity law. A uniaxial tension test was simulated in Abaqus/Explicit to compere experimental and numerical results.

Keywords
Constitutive model, plasticity, phase transformation, cryogenic temperature

1. Introduction

The present paper is focused on the constitutive description of FCC *(face centered cubic)* materials applied at very low temperatures. The theoretical description addresses two phenomena: plastic flow and austenite to martensite ($\gamma \rightarrow \alpha'$) phase transformation.

Phase transformation can be defined as a change in macroscopic configuration of atoms or molecules caused by change of thermodynamic variables characterizing the system, such as temperature, pressure or magnetic field. A phase is understood here as homogeneous microstructure, having homogeneous properties and defined boundaries. It is assumed here that $\gamma \rightarrow \alpha'$ transformation is the change of crystallographic configuration but without the diffusion mechanism. The plastic strain induced phase transformation is at the origin of considerable evolution of material properties (strong hardening).

The classical model of plastic strain induced $\gamma \rightarrow \alpha'$ phase transformation at low temperatures developed by Olson and Cohen (1975), attributes the onset of transformation to the intersection of shear bands. The authors have postulated for the so called TRIP steels a three parameter model capable of describing the experimentally verified sigmoidal curve that represents the volume fraction of martensite as a function of plastic strain. However, at very low temperatures the rate of phase transformation for a LSFE *(low stacking fault energy)* material becomes less temperature dependent and can be described by a simplified linearized model proposed by Garion and Skoczeń (Garion and Skoczeń 2002). Since the α'-martensite behaves in the flow range of austenite-martensite composite mostly in elastic way (yield point of α'-martensite is much higher than the yield point of γ-austenite (Sun X et al. 2009), its presence in the austenitic lattice affects the plastic flow and the process of hardening.

The constitutive model has been implemented in well-known FEM program Abaqus/Explicit with the use of user procedure VUMAT. The correlation between numerical and experimental results was performed to prove the correctness of the proposed model.

2. Constitutive description of the material

We consider a material that is susceptible to two coupled dissipative phenomena: plasticity and phase transformation, that are formalized on the macroscopic level by the use of a proper set of state variables. The motions within the considered thermodynamic system obey the fundamental laws of continuum mechanics (conservation of mass, conservation of linear momentum, conservation of angular momentum) and two laws of thermodynamics, written here in the local form:

- conservation of energy

$$\rho\dot{u} - \dot{\varepsilon}_{ij}\sigma_{ij} - r + q_{i,i} = 0 \tag{1}$$

Clausius-Duhem inequality

- $$\pi = -\rho(\dot{\psi} + s\dot{\theta}) + \dot{\varepsilon}_{ij}\sigma_{ij} - q_i \frac{\theta_{,i}}{\theta} \geq 0 \tag{2}$$

where π denotes the rate of dissipation per unit volume, ρ is the mass density per unit volume; σ_{ij} are the components of the stress tensor; u stands for the internal energy per unit mass; ε_{ij} denote the components of the total strain tensor; r is the distributed heat source per unit volume; q_i is the outward heat flux; s denotes the internal entropy production per unit mass, ψ stands for Helmholtz' free energy and θ is the absolute temperature.

The RVE based constitutive model presented in the paper is based on the following assumptions (Egner and Skoczeń, 2010):

- the martensitic platelets are randomly distributed and randomly oriented in the austenitic matrix,
- rate independent plasticity is assumed, because the influence of the strain rate $\dot{\varepsilon}_{ij}^{p}$ is small for the considered range of temperatures (2-77 K) (cf. Hecker et al., 1982),
- small strains are assumed: the accumulated plastic strain p does not exceed 0.2,
- mixed isotropic/kinematic plastic hardening affected by the presence of martensite fraction is included,
- the two-phase material obeys the associated flow rule (volume fraction of new phase not exceeding 0.5),
- isothermal conditions are considered (no fluctuations of temperature are taken into account).

Applying infinitesimal deformation theory to elastic – plastic – two phase material the total strain ε_{ij} can be expressed as a sum of the elastic part ε_{ij}^{e}, plastic ε_{ij}^{p}, and bain strain $\varepsilon^{bs} = \frac{1}{3}\Delta\upsilon\mathbf{I}$, denoting the additional strain caused by phase transformation.

$$\varepsilon_{ij} = \varepsilon_{ij}^{e} + \varepsilon_{ij}^{p} + \xi\varepsilon_{ij}^{bs} \tag{3}$$

The presented model is based on the framework of thermodynamics of irreversible processes with internal state variables, where Helmholtz free energy ψ is postulated as a state potential. The state potential depends on the elastic part of the total strain, and set of internal state variables, $\alpha_{ij}^{p}, r^{p}, \xi$, which define the current state of the material (Egner 2013, Egner and Ryś 2013):

$$\psi = \psi(\varepsilon_{ij}^{e}, \alpha_{ij}^{p}, r^{p}, \xi) \tag{4}$$

where $\alpha_{ij}^{p}, r^{p}, \xi$ are internal state variables describing the kinematic hardening, isotropic hardening and volume fraction of martensite, respectively.

The Helmholtz free energy of the material can be written as a sum of elastic (E), inelastic (I) and chemical (CH) terms (Abu Al-Rub and Voyiadjis, 2003; Egner, 2013):

$$\rho\psi = \rho\psi^{E} + \rho\psi^{I} + \rho\psi^{CH} \tag{5}$$

In the present model the following functions for $\rho\psi^{E}$ and $\rho\psi^{I}$ are assumed after Egner (2013):

$$\rho\psi^{E} = \frac{1}{2}\varepsilon_{ij}^{e} E_{ijkl}\varepsilon_{kl}^{e} \tag{6}$$

$$\rho\psi^{I} = \frac{1}{3}C^{p}\alpha_{ij}^{p}\alpha_{ij}^{p} + R_{\infty}^{p}\left[r^{p} + \frac{1}{b^{p}}exp\left(-b^{p}r^{p}\right)\right] \tag{7}$$

Term $\rho\psi^{CH}$ in Eq. (5) represents the chemically stored energy:

$$\rho\psi^{CH} = (1-n)\rho\psi_{\gamma}^{CH} + n\rho\psi_{\alpha'}^{CH} \tag{8}$$

where n is a function of martensite content such that $n(0)=0$ and $n(1)=1$ and define general mixture rule. The terms $\rho\psi_{\gamma}^{CH}$ and $\rho\psi_{\alpha'}^{CH}$ are the chemical energies of the respective phases, cf. Hallberg et al. (2010), Mahnken and Schneidt (2010). This internally stored energy is different for the two phases and it will affect the generation of heat during phase transformation, as well as the transformation itself.

Using the Clausius-Duhem inequality for isothermal case, one obtains:

$$\Pi^{mech} = \sigma_{ij}\dot{\varepsilon}_{ij} - \rho\dot{\psi} \geq 0 \tag{9}$$

where Π^{mech} is defined as mechanical dissipation.

Taking time derivative of Eq. (4) and using Clausius'a-Duhem (Eq. 9) inequality the following equations of thermodynamical forces are obtained:

$$\sigma_{ij} = \rho\frac{\partial\psi}{\partial\varepsilon_{ij}^{e}} = E_{ijkl}\varepsilon_{kl}^{e} = E_{ijkl}\left(\varepsilon_{kl} - \varepsilon_{kl}^{p} - \xi\varepsilon_{kl}^{bs}\right) \tag{10}$$

$$X_{ij}^{p} = \rho\frac{\partial\psi}{\partial\alpha_{ij}^{p}} = \frac{2}{3}C^{p}\alpha_{ij}^{p} \tag{11}$$

$$R^{p} = \rho\frac{\partial\psi}{\partial r^{p}} = R_{\infty}^{p}\left[1 - exp\left(-b^{p}r^{p}\right)\right] \tag{12}$$

$$Z = \rho\frac{\partial\psi}{\partial\xi} = \rho\frac{\partial\psi^{I}}{\partial\xi} + \frac{dn}{d\xi}\left(\rho\psi_{\alpha'}^{CH} - \rho\psi_{\gamma}^{CH}\right) \tag{13}$$

where X_{ij}^{p}, R^{p} and Z are the thermodynamic forces conjugated to the state variables α_{ij}^{p}, p and ξ, respectively.

It is assumed here that all dissipative mechanisms are governed by plasticity with a single dissipation potential F (Lemaitre 1992):

$$F\left(J_{cf}, N_{k}\right) = F^{p}\left(\sigma_{ij}, X_{ij}^{p}, R^{p}, \xi\right) + F^{tr}\left(Q, \xi\right) \tag{14}$$

Plastic potential F^{p} is here equal to von Mises type yield surface:

$$F^{p} = f^{p} = J_{2}\left(\sigma_{ij} - X_{ij}^{p}\right) - \sigma_{y} - R^{p} = 0 \tag{15}$$

and the phase transformation dissipation potential is assumed here in a simple form:

$$F^{tr} = AQ - B^{tr} = 0 \tag{16}$$

The quantity $Q = \sigma_{ij}\varepsilon_{ij}^{bs} - Z$ is conjugated to the transformation rate ξ and can be treated as a thermodynamic force that drives the phase front through the material (cf. Hallberg et al., 2007, 2010), $A(\theta, \sigma_{ij}, \dot{\varepsilon}_{ij}^{p})$, in general, is a function of temperature, stress state and strain rate, and B^{tr} is the barrier force for phase transformation (cf. Mahnken and Schneidt, 2010; Fisher et al., 2000). For rate independent plasticity, isothermal process and small stress variations function A may be treated as a constant value.

Normality rule involves only one plastic multiplier, determined from the consistency condition. The equations involving the dissipation potentials take the form:

$$\dot{\varepsilon}_{ij}^{p} = \dot{\lambda}^{p} \frac{\partial F^{p}}{\partial \sigma_{ij}} = \dot{\lambda}^{p} \frac{\partial f^{p}\left(\sigma_{kl}, X_{kl}^{p}, R^{p}\right)}{\partial \sigma_{ij}} = \dot{\lambda}^{p} \frac{\frac{3}{2}\left(s_{ij} - X_{ij}^{p}\right)}{\sqrt{\frac{3}{2}\left(s_{pq} - X_{pq}^{p}\right)\left(s_{pq} - X_{pq}^{p}\right)}} \tag{17}$$

$$\dot{\alpha}_{ij}^{p} = -\dot{\lambda}^{p} \frac{\partial F^{p}}{\partial X_{ij}^{p}} = \dot{\varepsilon}_{ij}^{p} \tag{18}$$

$$\dot{r}^{p} = -\dot{\lambda}^{p} \frac{\partial F^{p}}{\partial R^{p}} = \dot{\lambda}^{p} \tag{19}$$

$$\dot{\xi} = \dot{\lambda}^{p} \frac{\partial F^{tr}}{\partial Q} = A\, \dot{p} H\left[\left(p - p_{\xi}\right)\left(\xi_{L} - \xi\right)\right] \tag{20}$$

The consistency multiplier $\dot{\lambda}^{p}$ is obtained from the consistency condition:

$$\dot{f}^{p} = \frac{\partial f^{p}}{\partial \sigma_{ij}}(\dot{\sigma}_{ij} - \dot{X}_{ij}^{p}) + \frac{\partial f^{p}}{\partial R^{p}} \dot{R}^{p} + \frac{\partial f^{p}}{\partial \xi} \dot{\xi} = 0 \tag{21}$$

The evolution equations for thermodynamic conjugated forces are obtained by taking time derivatives of quantities defined by equations 10 -13. In particular, the force rates appearing in consistency condition (Eq. 21) are given by the following formulae:

$$\dot{\sigma}_{ij} = E_{ijkl}\left(\dot{\varepsilon}_{kl} - \dot{\varepsilon}_{kl}^{p} - \dot{\xi}\varepsilon_{kl}^{bs}\right) \tag{22}$$

$$\dot{X}_{ij}^{p} = \frac{2}{3} C^{p} \dot{\varepsilon}_{ij}^{p} + \frac{1}{C^{p}} \frac{\partial C^{p}}{\partial \xi} X_{ij}^{p} \dot{\xi} \tag{23}$$

$$\dot{R}^{p} = b^{p}\left(R_{\infty}^{p} - R^{p}\right)\dot{r}^{p} + \left[\frac{1}{R_{\infty}^{p}} \frac{\partial R_{\infty}^{p}}{\partial \xi} R^{p} + \left(R_{\infty}^{p} - R^{p}\right) r^{p} \frac{\partial b^{p}}{\partial \xi}\right]\dot{\xi} \tag{24}$$

where R_{∞}^{p}, b^{p}, C^{p} are a functions of ξ and, in the present paper, are assumed in the following form: $R_{\infty}^{p}(\xi) = R_{\infty,0}^{p}(1 + h_{R}\xi)$, $b^{p}(\xi) = b_{0}^{p}(1 + h_{b}\xi)$, $C^{p}(\xi) = C_{0}^{p}(1 + h_{C}\xi)$.

3. Numerical implementation

The derived constitutive model was implemented into Abaqus/Explicit by the use of VUMAT procedure and used to numerically simulate the behaviour of steel structural elements at cryogenic temperatures. At first the procedure in Wolffram Mathematica program was built to compare numerical (at Gauss point) and experimental results. After obtaining a good agreement of the results the procedure has been adopted to the finite element code Abaqus/Explicit by means of the user subroutine VUMAT written in FORTRAN. The VUMAT subroutine was adopted with the use of AceGen program which exports procedures written in Mathematica to FORTRAN automatically.

Application of the explicit dynamic procedure to quasi-static problems requires some special care. The goal is to simulate the process in the shortest possible time period in which inertial forces remain insignificant. Time increments of the order 10^{-9} [s] were used to satisfy the stability criteria. The algorithm, where Newton-Raphson scheme is used to solve the set of nonlinear equations (Eq. 20, 22-24), is shown in Table 1.

Table 1. Numerical alghorithm

Direct method
Backward Euler Scheme

(implicit)

1. Start with stored known variables:

$\left\{X_{ij}^{n}, R^{n}, \sigma_{ij}^{n}, \varepsilon_{ij}^{p,n}, \varepsilon_{ij}^{e,n}, \xi^{n}\right\}$ An increment of strain gives $\varepsilon_{ij}^{n+1} = \varepsilon_{ij}^{e,n} + \Delta\varepsilon_{ij}$.

2. Compute the elastic trial stress, the trial value for the yield function and test for plastic loading.

$$\sigma_{ij}^{trial} = \sigma_{ij}^{n} + E_{ijkl}\Delta\varepsilon_{kl}$$

$$f^{trial}(\sigma_{ij}^{trial}, X_{ij}^{n}, R^{n}, \xi^{n}) = 0$$

3. IF $f^{trial} \le 0$ then the load step is elastic

$$\sigma_{ij}^{n+1} = \sigma_{ij}^{trial}$$

$$\varepsilon_{ij}^{e,n+1} = \varepsilon_{ij}^{e,n} + \Delta\varepsilon_{ij}$$

EXIT the algorithm

4. IF $f^{trial} > 0$ then the load step is inelastic

The residual vector is defined as:

$\mathbf{R} = \left[R_{(\sigma)ij}, R_{(X)ij}, R_{R}, R_{f}, R_{\xi}\right]^{T}$, where

$$R_{(\sigma)ij} = \sigma_{ij} - \sigma_{ij}^{old} - E_{ijkl}^{old}\left(\Delta\varepsilon_{kl} - \frac{\partial f^{p,new}}{\partial\sigma_{kl}}\Delta\lambda^{p} - \Delta\xi\varepsilon_{kl}^{bs}\right)$$

$$R_{(X)ij} = X_{ij}^{p} - X_{ij}^{p,old} - \frac{2}{3}C^{p,new}\frac{\partial f^{p,new}}{\partial\sigma_{ij}}\Delta\lambda^{p}$$

$$R_{(R)} = R^{p} - R^{p,old} - b^{p,new}\left(R_{\infty}^{p,new} - R^{p,old}\right)\Delta p$$

$$R_{f} = f^{p}$$

$$R_{\xi} = \xi - \xi^{old} - \Delta\xi$$

and the vector of unknowns is defined as

$$\mathbf{U} = \left[\sigma_{ij}, X_{ij}^{p}, R^{p}, \Delta\lambda^{p}, \xi\right]^{T}$$

The condition $\mathbf{R}(\mathbf{U}) = \mathbf{0}$ defines the solution of the problem. The solution can be reached with the use of following iteration procedure with condition $\mathbf{R}(\mathbf{U}) = error$, where error is defined by the user.

1. Initialize

$$\mathbf{U}_{n+1}^{(0)} = \mathbf{U}_{n}$$

$$\mathbf{U}^{new(0)} = \mathbf{U}^{old}$$

2. Iterate

$$\text{DO UNTIL } \left\|\mathbf{R}(\mathbf{U}^{(k)})\right\| < TOL$$

$$k \leftarrow k+1$$

2.1 Compute iteration $\mathbf{U}^{(k+1)}$

$$\mathbf{U}^{(k+1)} = \mathbf{U}^{(k)} - \left[\frac{\partial\mathbf{R}^{(k)}}{\partial\mathbf{U}}\right]^{-1}\mathbf{R}(\mathbf{U}^{(k)})$$

2.2 Update $\mathbf{U}$

$$\mathbf{U}_{n+1}^{new} = \mathbf{U}^{(k+1)}$$

EXIT

At first, a two-dimensional initial boundary value problem was considered. A specimen of length 100 mm was fixed on one side and free on the other side. The mesh discretization of 5x10 elements was used (Fig.1 right).
Accounting for two dissipative phenomena: plasticity and phase transformation in the present constitutive model allows to obtain a satisfactory reproduction of the experimental stress-strain curve for 316L stainless steel subjected to uniaxial tension at cryogenic temperatures (see Fig. 1). A small difference between numerical and experimental results is caused by damage which is not included in the present model.

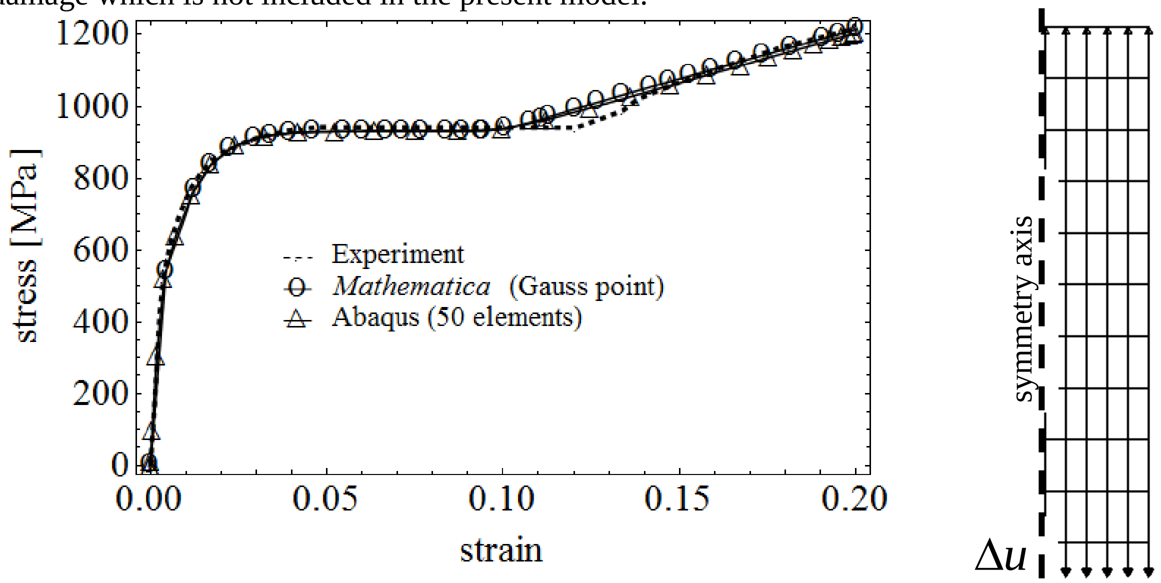

Fig. 1. Stress-strain curve for 316L stainless steel at 4.2K (left), model implemented in Abaqus/Explicit (right)

Thanks to the implementation in the finite element software of the constitutive model of a material undergoing the plastic strain-induced phase transformation, the mechanical behavior of any structure can be easily computed and the evolution of two-phase continuum created during the transformation can be investigated. As an example, the finite element analysis of expansion bellows is presented.
Bellows expansion joints belong to thin-walled structures of high flexibility. They are used to compensate for the relative motion of two adjacent assemblies subjected to the loads. The bellows expansion joints are crucial elements for systems working at cryogenic temperatures, where all structures contract significantly during cool-down process and the emerging displacement of components need to be compensated. Several examples of bellows expansion joints are shown in Fig. 2.

Fig. 2. Examples of bellows expansion joints in the LHC accelerator (CERN) (Sitko 2011)

The finite element model has been built by means of CAX4R (4-node bilinear axisimmetric quadrilateral) elements assuming the axial symmetry. Moreover, it has been assumed that the expansion bellows is made of 316L stainless steel and is modelled for the conditions of liquid helium (4.2K). The implemented geometry and mesh is shown in Fig. 3.

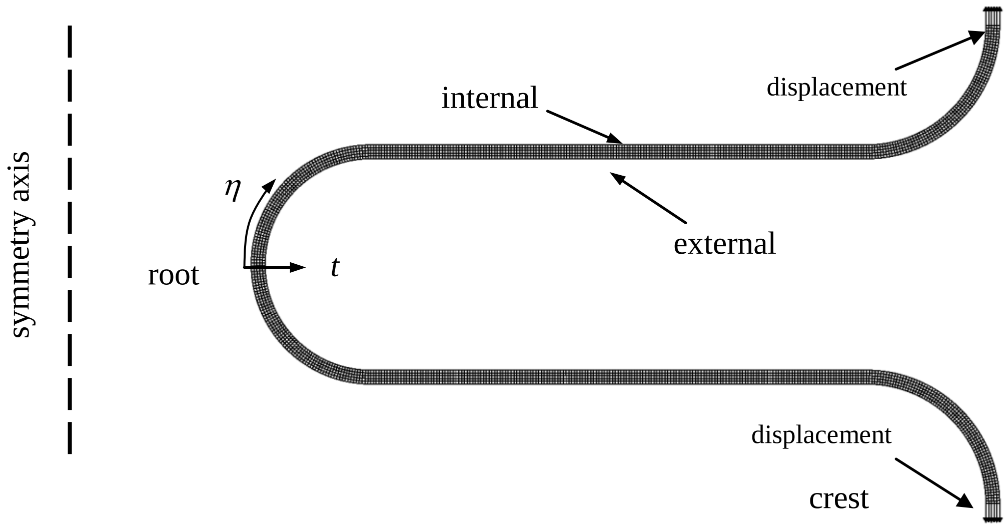

Fig. 3. Boundary conditions and finite element mesh of expansion bellows

The intensity of the martensitic transformation is maximal at root and at crest of the bellows, due to the localisation of the plastic strains (Fig. 4.).

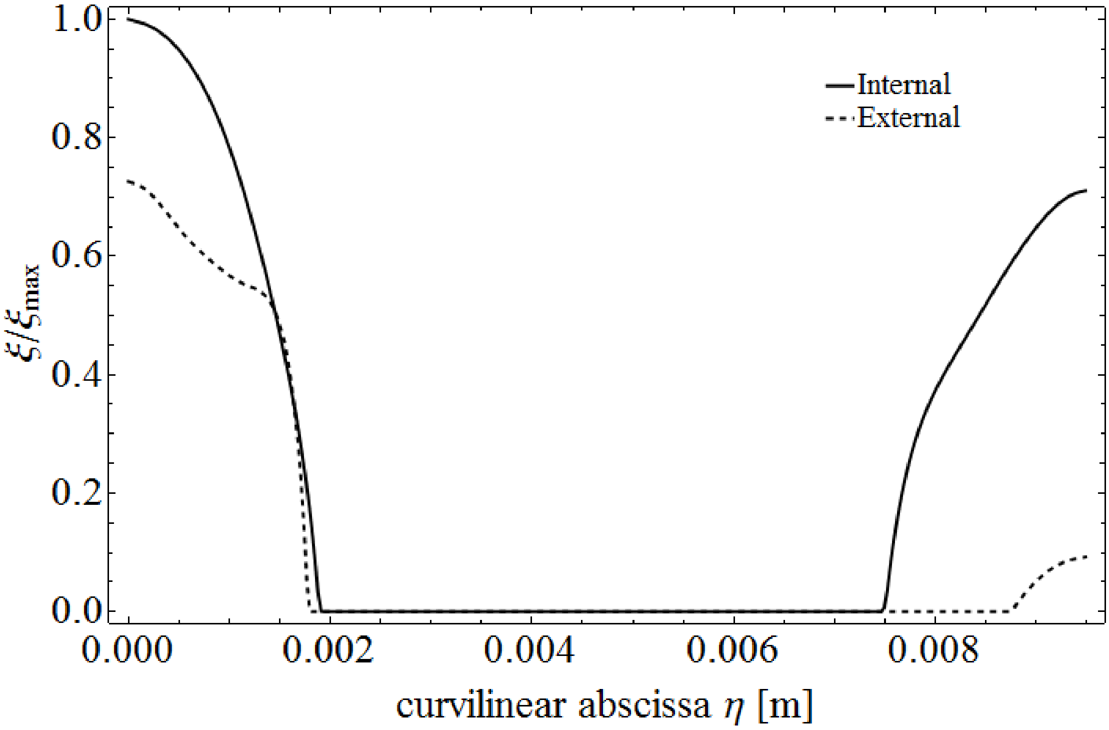

Fig. 4. Distribution of martensitic phase along the curvilinear abscissa η *(external and internal side, see Fig.3.)*

4. Conclusions

The constitutive model presented in the paper includes two dissipative phenomena: plastic yielding and plastic strain induced phase transformation. A consistent thermodynamic framework was used in order to describe these phenomena. The Garion-Skoczeń model was used as the kinetic law of phase transformation. The model was implemented in the explicit finite element code Abaqus/Explicit by means of the user subroutine VUMAT. A uniaxial tension simulation of the bar was made to prove the correctness of the model. The constitutive model was then applied to the numerical analysis of thin-walled stainless steel corrugated shells, known as bellows expansion joints.

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