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CONSTITUTIVE MODELLING OF DAMAGE EVOLUTION AND MARTENSITIC TRANSFORMATION IN 316L STAINLESS STEEL

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Abstract: In this work, the constitutive model, derived with the use of thermodynamic of irreversible processes framework is presented. The model is derived under the assumption of small strains. Plastic strain induced martensitic phase transformation is considered in the austenitic matrix where the volume fraction of the martensite is reflected by a scalar parameter. The austenitic matrix is assumed as the elastic-plastic material and martensitic phase is assumed as randomly distributed and randomly oriented inclusions. Both phases are affected by damage evolution but there is no distinction in the model between damage in austenite and martensite.

Key word: Constitutive Modelling, Dissipative Materials, Phase Transformation, Damage Evolution

1. INTRODUCTION

In this work a material that is susceptible to several coupled dissipative phenomena: plasticity, damage, and phase transformation, that are formalized on the macroscopic level by the use of a proper set of state variables, is considered. Other phenomena, like discontinuous yielding are not taken into account here (Egner and Skoczeń 2010, Skoczeń et al., 2014).

Among metallic materials, that are characterized by the mentioned above dissipative phenomena, we can find austenitic stainless steels. These materials preserve ductility practically down to 0K, thus they are applied for components of superconducting magnets and cryogenic transfer lines: tubes, cylinders, thin walled shells (like bellows expansion joints) or massive parts like vacuum barriers (Ryś, 2015). In the present paper 316L stainless steel is chosen as a field of application of the constitutive description.

The first model of plastic strain induced austenite to martensite ($\gamma \rightarrow \alpha'$) phase transformation was proposed by Olson and Cohen (1975). The authors, on the basis of micromechanical observations, developed 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. Later on, this model was widely used by others (Stringfellow et al., 1992; Tomita and Iwamoto, 2001; Iwamoto, 2004). Moreover, Stringfellow et al., (1992) expanded on Olson and Cohen's law by incorporating the effect of stress triaxiality on the phase transformation. Tomita and Iwamoto (1995) generalized the model proposed by Stringfellow et al., (1992) by taking into account the effect of strain rate. Micromechanical model was developed by Diani et al. (1995) and later on Cherkaoui et al. (1998) proposed a micromechanical model of martensitic transformation induced plasticity in austenitic single crystal. Another micromechanical model was proposed by Fischer and Schlögl (1995), the Authors investigated the local stress state in a martensitically transforming micro-region including plastic anisotropy. In the paper published by Fischer et al. (2000) the authors devoted their attention to explanation of the martensitic transformation in polycrystalline materials subjected to non-proportional loading paths. A simple phenomenological stress independent transformation law to describe the deformation – induced martensite formation in stainless steel was also proposed by Santacreu et al. (2006). Santacreu's et al. model was further generalized by Beese and Mohr (2011) who proposed a stress-state-dependent transformation kinetics law that incorporates the effect of the Lode angle parameter in addition to the stress triaxiality. However, in the present work the Santacreu's et al. (2006) model in his basic form is chosen to use.

Other constitutive models of materials undergoing phase transformation are due to: Narutani et al. (1982); Cherkaoui et al. (2000); Fischer and Reisner (1998); Diani and Parks (1998); Levitas et al. (1999); Heung Nam Han et al. (2004); Kubler et al. (2011); Ziętek and Mróz (2011), and many others.

In contrast to the beneficial properties, martensitic transformations may also have a detrimental effect on the thermomechanical response of a material. This occurs if the martensitic product phase is relatively hard and brittle, and provides nucleation sites for crystalline damage. Moreover, crystalline damage eventually may lead to crack formation at a higher length scale.

There exists some evidence for the presence of micro-damage fields within the martensite sites (cf Baffie et al., 2000; Le Pecheur, 2008). It seems that the bain strain, associated with formation of the martensite inclusions, can promote local development of damage fields. Also, the martensite platelets are supposed to be carriers of the short cracks that contribute to the general state of damage (see Fig. 2). For this reason the evolution of damage fields has been postulated both in the matrix and in the inclusions. However, there is no distinction between the type of damage in austenite and martensite in the model. Thus, the average content of damage in the RVE (representative volume element) is described by one single scalar parameter. This simpli-

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fication is strong because martensitic phase is hard and behaves rather like rock-like material (Egner et al. 2015a, Stolarz 2001). However, it is very difficult to estimate damage content in each phase separately, what justifies the above assumption. On the other hand, as the boundaries between the inclusions and the matrix are coherent, the micro-damage related to some sort of delamination or decohesion within the boundaries has not been taken into account.

For other approaches of damage modeling in austenitic steels see Suiker and Turteltaub (2006, 2007); Egner et al., (2015a, b); Garion and Skoczeń (2003).

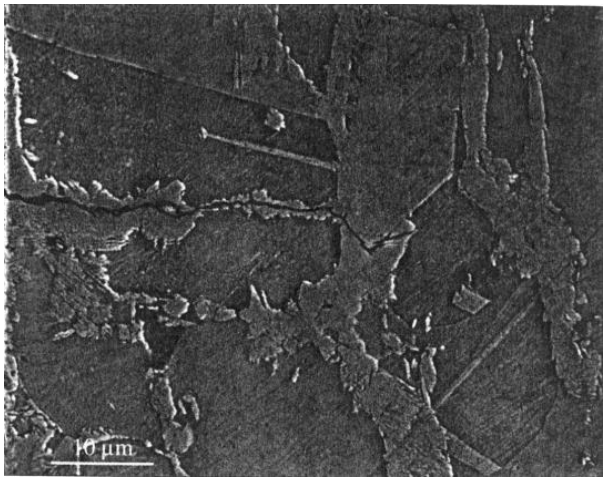

Fig. 1. Propagation of a short crack across an island of martensite (Baffie et al., 2000)

As was mentioned above, the scalar damage parameter, D (with condition: $D = 0$ – initial undamaged state, $D = 1$ – final fractured state), is used to reflect the damage state in the RVE. This concept was proposed first by Kachanov (1958) and then modified by Rabotnov (1968, 1969), and may be interpreted as the fraction of decrease in the effective area due to damage development (Murakami, 2012). In the constitutive modelling damage parameter is used to take into account the influence of voids and cracks accumulation in material on the stress concentration and reduction of the stiffness of the material.

The classical laws of kinematic and isotropic hardening are postulated in the present work. Since the phase transformation has strong influence on hardening process during the plastic deformation, the volume fraction of martensite affects the parameters of both kinematic and isotropic hardening. The kinetic laws for state variables are derived from the normality rule applied to the plastic potential, while the consistency multiplier is obtained from the consistency condition applied to the yield function (Chaboche 2008).

2. CONSTITUTIVE DESCRIPTION OF THE ELASTIC-PLASTIC-DAMAGE TWO PHASE MATERIAL

The author considers a material that is susceptible to three coupled dissipative phenomena: plasticity, damage evolution and phase transformation. 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

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

— Clausius-Duhem inequality

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

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 (see also Egner et al. 2015 a,b; Ryś, 2014):

— the martensitic platelets are randomly distributed and randomly oriented in the austenitic matrix,
— both phases are affected by damage,
— rate independent plasticity is assumed,
— small strains are assumed,
— mixed isotropic/kinematic plastic hardening affected by the presence of martensite fraction is included,
— isothermal conditions are considered.

Applying infinitesimal deformation theory to elastic – plastic – damage - 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 $\epsilon^{bs} = 1/3\Delta v I$, denoting the additional strain caused by phase transformation.

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

In order to include in the model variation of the material properties caused by the damage development the mechanical behavior of a damaged material is usually described by using the notion of the effective state variables, together with the hypothesis of mechanical equivalence between the damaged and undamaged configuration.

The current state in representative volume element (RVE) of a real, damaged configuration, $\mathrm{B_t}$, (Fig 1a) is specified by the pairs of state variables:

$$\left(\sigma_{ij}, \epsilon_{ij}^e\right), \left(R^p, r^p\right), \left(X_{ij}^p, \alpha_{ij}^p\right), (Z, \xi), (-Y, D) \tag{4}$$

It is also assumed the exisctence of the fictitious undamaged configuration, B_f, (Fig 1b) which has the identical total strain energy W_T to that of B_t and hence is mechanically equivalent to B_t (Saanouni et. al, 1994, Murakami, 2012).

It is assumed further that the mechanical state of the RVE in fictitious undamaged configuration is described by the set of the effective variables corresponding to Eq. 7.

$$\left(\tilde{\sigma}_{ij}, \tilde{\epsilon}_{ij}^e\right), \left(\tilde{R}^p, \tilde{r}^p\right), \left(\tilde{X}_{ij}^p, \tilde{\alpha}_{ij}^p\right), (Z, \xi), (Y = 0, D = 0) \tag{5}$$

Thus, the hypothesis of total energy equivalence employed in the present work can be formulated as: The mechanical behaviour of a damaged material in the current damaged configuration B_t (Fig 2a) is derived from state and dissipation potentials defined in the fictitious undamaged configuration B_f (Fig 2b) by repleacing the state variables in them by the corresponding effective state

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variables (Saanouni et al., 1994; Murakami, 2012; Saanouni, 2012).

Accordingly, the application of this energy equivalence principle leads to:

$$W_T\left(\epsilon_{ij}^e; \alpha_{ij}^p, r^p, \xi, D\right) = W_T(\tilde{\epsilon}_{ij}^e; \tilde{\alpha}_{ij}^p, \tilde{r}^p, \xi, D = 0) \tag{6}$$

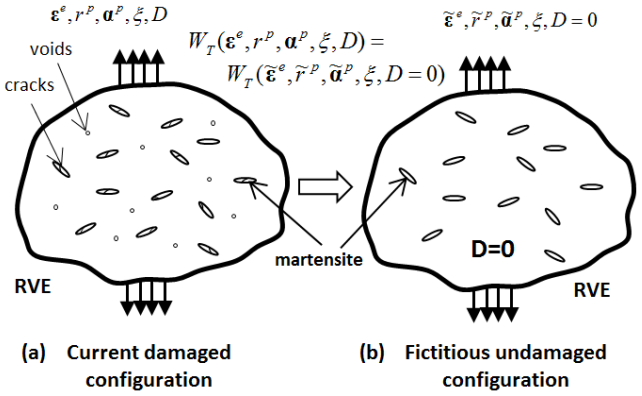

Fig. 2. Hypothesis of total energy equivalence

Since the total energy W_T can be devided into elastic part W_E and parts corresponding to kinematic W_K and isotropic W_I hardening the following relations should be satisfied (Murakami, 2012, Saanouni, 2012):

$$W_E\left(\epsilon_{ij}^e, D\right) = W_E\left(\tilde{\epsilon}_{ij}^e, D = 0\right) = \frac{1}{2}\sigma_{ij}\epsilon_{ij}^e = \frac{1}{2}\tilde{\sigma}_{ij}\tilde{\epsilon}_{ij}^e \tag{7}$$

$$W_K\left(\alpha_{ij}^p, D\right) = W_K\left(\tilde{\alpha}_{ij}^p, D = 0\right) = \frac{1}{2}X_{ij}^p\alpha_{ij}^p = \frac{1}{2}\tilde{X}_{ij}^p\tilde{\alpha}_{ij}^p \tag{8}$$

$$W_I(r^p, D) = W_I(\tilde{r}^p, D = 0) = \frac{1}{2}R^p r^p = \frac{1}{2}\tilde{R}^p\tilde{r}^p \tag{9}$$

It is worth to point it out that phase transformation is assumed here not affected by the damage evolution.

The above relations (Eq. 7 - 9) are always satisfied if the effective state variables are defined as follows (Murakami, 2012, Saanouni, 2012):

$$\tilde{\sigma}_{ij} = \frac{\sigma_{ij}}{\sqrt{(1-D)}}, \tilde{\epsilon}_{ij}^e = \sqrt{(1-D)}\epsilon_{ij}^e \tag{10}$$

$$\tilde{X}_{ij}^p = \frac{X_{ij}^p}{\sqrt{(1-D)}}, \tilde{\alpha}_{ij}^p = \sqrt{(1-D)}\alpha_{ij}^p \tag{11}$$

$$\tilde{R}^p = \frac{R^p}{\sqrt{(1-D)}}, \tilde{r}^p = \sqrt{(1-D)}r^p \tag{12}$$

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 ϵ_{ij}^e of the total strain ϵ_{ij}, and set of internal state variables $\{\alpha_{ij}^p, r^p, \xi, D\}$, which define the current state of the material:

$$\psi = \psi(\epsilon_{ij}^e; \alpha_{ij}^p, r^p, \xi, D) \tag{13}$$

where $\alpha_{ij}^p, r^p, \xi, D$ are variables related to the kinematic hardening, isotropic hardening, volume fraction of martensite and damage parameter, respectively. Moreover, the damage parameter, D, reflects the average state of damage in whole RVE. There is also the assumption of the existence of thermodynamic forces corresponding to the internal variables

$$\{X_{ij}^p, R^p, Z, -Y\} \tag{14}$$

where $X_{ij}^p, R^p, Z, -Y$ denote, respectively, kinematic and isotropic hardening conjugated forces, thermodynamic conjugated force associated to phase transformation and the associated thermodynamic conjugated force with the isotropic damage variable D.

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 et al., 2015a):

$$\psi = \psi^E + \psi^I + \psi^{CH} \tag{15}$$

In the present paper the Helmholtz free energy (Eq. 6) is a quadratic function of all of the strain-like variables and in the fictive configuration it is formulated as (Saanouni, 2012, Besson et. al, 2010):

$$\psi^E = \frac{1}{2}\tilde{\epsilon}_{ij}^e E_{ijkl}\tilde{\epsilon}_{kl}^e = \frac{1}{2}(1-D)\epsilon_{ij}^e E_{ijkl}\epsilon_{kl}^e \tag{16}$$

$$\psi^I = \frac{1}{3}C^p(\xi)\tilde{\alpha}_{ij}^p\tilde{\alpha}_{ij}^p + \frac{1}{2}R_\infty^p(\xi)(\tilde{r}^p)^2 = \frac{1}{3}(1-D)C^p(\xi)\alpha_{ij}^p\alpha_{ij}^p + \frac{1}{2}(1-D)R_\infty^p(\xi)(r^p)^2 \tag{17}$$

Term ψ^{CH} in Eq. 15 represents the chemically stored energy:

$$\psi^{CH} = (1-\xi)\psi_\gamma^{CH} + \xi\psi_{\alpha'}^{CH} \tag{18}$$

The terms ψ_γ^{CH} and $\psi_{\alpha'}^{CH}$ 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:

$$\pi^{mech} = \sigma_{ij}\dot{\epsilon}_{ij} - \dot{\psi} \geq 0 \tag{19}$$

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

The time derivative of Helmholtz free energy (Eq. 15) as a function of internal state variables is given by:

$$\dot{\psi} = \frac{\partial\psi}{\partial\epsilon_{ij}^e}\dot{\epsilon}_{ij}^e + \frac{\partial\psi}{\partial\alpha_{ij}^p}\dot{\alpha}_{ij}^p + \frac{\partial\psi}{\partial r^p}\dot{r}^p + \frac{\partial\psi}{\partial\xi}\dot{\xi} + \frac{\partial\psi}{\partial D}\dot{D} \tag{20}$$

Substituting the rate of the Helmholtz free energy into Clausius-Duhem inequality the following thermodynamic constraint is obtained:

$$\left(\sigma_{ij} - \frac{\partial\psi}{\partial\epsilon_{ij}^e}\right)\dot{\epsilon}_{ij}^e + \sigma_{ij}\dot{\epsilon}_{ij}^p - \frac{\partial\psi}{\partial\alpha_{ij}^p}\dot{\alpha}_{ij}^p - \frac{\partial\psi}{\partial r^p}\dot{r}^p - \frac{\partial\psi}{\partial\xi}\dot{\xi} - \frac{\partial\psi}{\partial D}\dot{D} \geq 0 \tag{21}$$

Eq. 21 results in the following thermodynamic state laws for the conjugate thermodynamic forces:

$$\sigma_{ij} = \frac{\partial\psi}{\partial\epsilon_{ij}^e} = (1-D)E_{ijkl}^0\left(\epsilon_{kl} - \epsilon_{kl}^p - \xi\epsilon_{kl}^{bs}\right) \tag{22}$$

$$X_{ij}^p = \frac{\partial\psi}{\partial\alpha_{ij}^p} = \frac{2}{3}(1-D)C^p(\xi)\alpha_{ij}^p \tag{23}$$

$$R^p = \frac{\partial\psi}{\partial r^p} = (1-D)R_\infty^p(\xi)r^p \tag{24}$$

$$Z = \frac{\partial\psi}{\partial\xi} = \rho\frac{\partial\psi^I}{\partial\xi} + \left(\rho\psi_{\alpha'}^{CH} - \rho\psi_\gamma^{CH}\right) \tag{25}$$

$$Y = -\frac{\partial\psi}{\partial D} = Y^E + Y^{IN} = \frac{1}{2}\epsilon_{ij}^e E_{ijkl}^0\epsilon_{kl}^e + \frac{1}{3}C^p(\xi)\alpha_{ij}^p\alpha_{ij}^p + \frac{1}{2}R_\infty^p(\xi)(r^p)^2 \tag{26}$$

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Thermodynamic force, Y, conjugated to the damage parameter, D, is the strain energy density release rate and in the case when the hypothesis of total energy equivalence is employed represents the contribution from elasticity, kinematic hardening, and isotropic strain hardening.

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

$$F = F^p\left(\sigma_{ij}, X_{ij}^p, R^p, \xi\right) + F^{TR}(Q,\xi) + F^D(-Y, D) \tag{27}$$

Plastic potential $\mathrm{F^p}$ has the following form:

$$F^p = f^p + \frac{1}{2}\frac{b}{R_\infty^p(\xi)}\left(\tilde{R}^p\right)^2 + \frac{1}{2}\frac{\gamma}{C^p(\xi)}\frac{3}{2}\tilde{X}_{ij}^p\tilde{X}_{ij}^p \tag{28}$$

where, $\mathrm{f^p}$ is von Mises yield function:

$$f^p = J_2\left(\tilde{\sigma}_{ij} - \tilde{X}_{ij}^p\right) - \sigma_y - \tilde{R}^p = \sqrt{\frac{3}{2}\left(\tilde{\sigma}_{ij}^D - \tilde{X}_{ij}^p\right)\left(\tilde{\sigma}_{ij}^D - \tilde{X}_{ij}^p\right)} - \sigma_y - \tilde{R}^p \tag{29}$$

where, $\tilde{\sigma}_{\mathrm{ij}}^{\mathrm{D}}$ is the deviatoric part of the Cauchy stress tensor.

The phase transformation dissipation potential is assumed here in the following form:

$$F^{TR} = \frac{1}{\sqrt{1-D}}(\xi^{max} - \xi)mA(Ap)^{m-1}Q^{TR} - B^{TR} \tag{30}$$

The quantity $\mathrm{Q^{TR}} = \sigma_{\mathrm{ij}}\epsilon_{\mathrm{ij}}^{\mathrm{bs}} - \mathrm{Z}$ is conjugated to the transformation rate $\dot{\xi}$ and can be treated as a thermodynamic force that drives the phase front through the material (cf. Hallberg et al., 2007, 2010), p is accumulated plastic strain, A, m, $\xi^{\max}$ are the model parameters that have to be found through experimental validation of the model, and $\mathrm{B^{tr}}$ is the barrier force for phase transformation (cf. Mahnken and Schneidt, 2010; Fisher et al., 2000).

Damage dissipation potential is as follows (Bonora, 1997):

$$F^D = \frac{1}{2}\frac{S}{\sqrt{1-D}}\left(\frac{Y}{S}\right)^2\frac{(D_C - D)^{(\alpha-1)/\alpha}}{p^{(n+2)/n}} \tag{31}$$

where $\mathrm{D_C}$ is the critical value of damage variable for which ductile failure occurs, S is a model parameter, n is the material hardening exponent, while α is an exponent characterizing the damage development.

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

$$\dot{\epsilon}_{ij}^p = \dot{\lambda}^p\frac{\partial F^p}{\partial \sigma_{ij}} = \frac{\dot{\lambda}^p}{\sqrt{1-D}}\frac{3}{2}\frac{\left(\sigma_{ij}^D - X_{ij}^p\right)}{J_2\left(\sigma_{ij}^D - X_{ij}^p\right)} \tag{32}$$

$$\dot{p} = \sqrt{\frac{2}{3}\dot{\epsilon}_{ij}^p\dot{\epsilon}_{ij}^p} = \frac{\dot{\lambda}^p}{\sqrt{1-D}} \tag{33}$$

$$\dot{\alpha}_{ij}^p = -\dot{\lambda}^p\frac{\partial F^p}{\partial X_{ij}} = \dot{\epsilon}_{ij}^p - \gamma\dot{\lambda}^p\alpha_{ij}^p = \dot{\epsilon}_{ij}^p - \gamma\dot{p}\sqrt{1-D}\alpha_{ij}^p \tag{34}$$

$$\dot{r}^p = -\dot{\lambda}^p\frac{\partial F^p}{\partial R^p} = \frac{\dot{\lambda}^p}{\sqrt{1-D}}\left(1 - b\sqrt{1-D}r^p\right) = \dot{p}\left(1 - b\sqrt{1-D}r^p\right) \tag{35}$$

$$\dot{\xi} = \dot{\lambda}^p\frac{\partial F^{TR}}{\partial Q^{TR}} = (\xi^{max} - \xi)mA(Ap)^{m-1}\dot{p} \tag{36}$$

It has to be mentioned here that the phase transformation dissipation employed in the form of Eq. 30 allows to obtain kinetic law of phase transformation orginally proposed by Santacreu et al. (2006).

The choice of the damage potential (Eq. 31) leads to the following damage kinetic evolution with the effective accumulated plastic strain (Bonora, 1997):

$$\dot{D} = \frac{\dot{\lambda}^p}{\sqrt{1-D}}\left(\frac{Y}{S}\right)\frac{(D_C - D)^{(\alpha-1)/\alpha}}{p^{(n+2)/n}} = Y\frac{(D_C - D)^{(\alpha-1)/\alpha}}{S}\frac{\dot{p}}{p^{(n+2)/n}} \tag{37}$$

Bonora in his works used the strain energy equivalence hypothesis which results, in accordance with symbols in the present article, that $\mathrm{Y = Y^E}$. In the case of isotropic material elastic part of Y can be expressed as a function of the von Mises equivalent stress σ_{EQ} and the stress triaxiality (defined as a ratio of the hydrostatic stress and von Mises stress, $\sigma_{\mathrm{H}}/\sigma_{\mathrm{EQ}}$) (Lemaitre, 1992; Murakami, 2012):

$$Y^E = \frac{(\sigma_{EQ})^2}{2E(1-D)^2}\left(\frac{2}{3}(1+\upsilon) + 3(1-2\upsilon)\left(\frac{\sigma_H}{\sigma_{EQ}}\right)^2\right) = \frac{(\sigma_{EQ})^2}{2E(1-D)^2}f\left(\frac{\sigma_H}{\sigma_{EQ}}\right) \tag{38}$$

Moreover, Bonora proposed to use the Ramberg – Osgood relation

$$p = \left(\frac{\sigma_{EQ}}{(1-D)K}\right)^n \tag{39}$$

what gives

$$\dot{D} = \frac{K^2}{2ES}f\left(\frac{\sigma_H}{\sigma_{EQ}}\right)(D_C - D_0)^{(\alpha-1)/\alpha}\frac{\dot{p}}{p} \tag{40}$$

It can be shown (Murakami, 2012) that integration of this relation under uniaxial tenstion with the initial condition of $\mathrm{p = \epsilon_D}$ and $\mathrm{D = D_0}$, and then applying the fracture condition $\epsilon = \epsilon_{\mathrm{R}}$, $\mathrm{D = D_C}$ one can obtain the reliation:

$$\frac{K^2}{2ES} = \alpha\frac{(D_C - D_0)^{1/\alpha}}{\ln(\epsilon/\epsilon_D)} \tag{41}$$

Finally, we can obtain the following kinetic equation of the damage evolution:

$$\dot{D} = \alpha\frac{(D_C - D_0)^{1/\alpha}}{\ln(\epsilon_f) - \ln(\epsilon_{th})}f\left(\frac{\sigma_m}{\sigma_{EQ}}\right)(D_C - D)^{(\alpha-1)/\alpha}\frac{\dot{p}}{p} \tag{42}$$

where, $\mathrm{D_0}$ is the initial damage state in the material microstructure, ϵ_{th} and ϵ_{f} are threshold strain at which damage process starts and the strain to failure in the uniaxial state of stress, respectively.

The use of the total energy equivalence, in the present work, imply that $\mathrm{Y = Y^E + Y^{IN}}$. Moreover, as denoted by Saanouni et al. (1994) the contribution of the inelastic part, $\mathrm{Y^{IN}}$, in the total damage energy release rate, Y, is significant and should not be neglected. Hence, in the present work, the basic form (Eq. 37) of the kinetic equation of the damage evolution is used in which the relation $\mathrm{Y = Y^E + Y^{IN}}$ is applied.

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

$$\dot{f}^p = \frac{\partial f^p}{\partial \sigma_{ij}}\left(\dot{\sigma}_{ij} - \dot{X}_{ij}^p\right) + \frac{\partial f^p}{\partial R^p}\dot{R}^p + \frac{\partial f^p}{\partial D}\dot{D} + \frac{\partial f^p}{\partial \xi}\dot{\xi} = 0 \tag{43}$$

The evolution equations for thermodynamic conjugated forces are obtained by taking time derivatives of quantities defined by equations 22 - 24. In particular, the force rates appearing in consistency condition (Eq. 43) are given by the following formulae:

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$$\dot{\sigma}_{ij} = E_{ijkl}(D)\left(\dot{\epsilon}_{kl} - \dot{\epsilon}^{p}_{kl} - \dot{\xi}\epsilon^{bs}_{kl}\right) - E^{0}_{ijkl}\left(\epsilon_{kl} - \epsilon^{p}_{kl} - \xi\epsilon^{bs}_{kl}\right)\dot{D} \quad (44)$$

$$\dot{X}^{p}_{ij} = \frac{2}{3}(1-D)C^{p}(\xi)\dot{\alpha}^{p}_{ij} - \left(\frac{\dot{D}}{1-D} - \frac{1}{C^{p}(\xi)}\frac{\partial C^{p}(\xi)}{\partial \xi}\dot{\xi}\right)X^{p}_{ij} \quad (45)$$

$$\dot{R}^{p} = (1-D)R^{p}_{\infty}(\xi)\dot{r}^{p} - \left(\frac{\dot{D}}{1-D} - \frac{1}{R^{p}_{\infty}(\xi)}\frac{\partial R^{p}_{\infty}(\xi)}{\partial \xi}\dot{\xi}\right)R^{p} \quad (46)$$

In the present work, the simplest, linear form of functions $C^{p}(\xi)$ and $R^{p}_{\infty}(\xi)$ is assumed, namely:

$$C^{p}(\xi) = C^{p}_{0}(1 + h_{C}\xi), \quad (47)$$

$$R^{p}_{\infty}(\xi) = R^{p}_{\infty,0}(1 + h_{R}\xi) \quad (48)$$

3. LOCAL INTEGRATION SCHEME

In the present work elastic predictor – plastic corrector procedure is used where the Newton-Raphson scheme is adopted to solve all nonlinear equations. Applying the forward Euler scheme, equations of time-independent plasticity, Eq. 32, 34-37 and 29 can be written in the following residual form:

$$R^{\epsilon}_{ij} = \epsilon^{p,n+1}_{ij} - \epsilon^{p,n}_{ij} - \frac{\Delta\lambda^{p}}{\sqrt{1-D^{n+1}}}\frac{3}{2}\frac{\left(\sigma^{D,n+1}_{ij} - X^{p,n+1}_{ij}\right)}{J_{2}\left(\sigma^{D,n+1}_{ij} - X^{p,n+1}_{ij}\right)} \quad (49)$$

$$R^{\alpha}_{ij} = \alpha^{p,n+1}_{ij} - \frac{1}{1+\gamma\Delta\lambda^{p}}\left(\alpha^{p,n}_{ij} + \Delta\epsilon^{p}_{ij}\right) \quad (50)$$

$$R^{r} = r^{p,n+1} - \frac{1}{1+b\Delta\lambda^{p}}\left(r^{p,n} + \frac{\Delta\lambda^{p}}{\sqrt{1-D}}\right) \quad (51)$$

$$R^{D} = D^{n+1} - D^{n} - \frac{\Delta\lambda^{p}}{\sqrt{1-D}}\left(\frac{Y^{n+1}}{S}\right)\frac{(D_{C} - D^{n+1})^{(\alpha-1)/\alpha}}{p^{(n+2)/n}} \quad (52)$$

$$R^{\xi} = \xi^{n+1} - \xi^{n} - (\xi^{max} - \xi^{n+1})mA(Ap)^{m-1}\frac{\Delta\lambda^{p}}{\sqrt{1-D}} \quad (53)$$

$$R^{f} = f^{p,n+1} = \frac{1}{\sqrt{1-D^{n+1}}}\sqrt{\frac{3}{2}\left(\sigma^{D,n+1}_{ij} - X^{p,n+1}_{ij}\right)\left(\sigma^{D,n+1}_{ij} - X^{p,n+1}_{ij}\right)} - \sigma_{y} - \frac{R^{p,n+1}}{\sqrt{1-D^{n+1}}} = 0 \quad (54)$$

The stress – like variables involved in the above equations are given by:

$$\sigma^{n+1}_{ij} = (1-D^{n+1})E^{0}_{ijkl}\left(\epsilon^{n+1}_{kl} - \epsilon^{p,n+1}_{kl} - \xi^{n+1}\epsilon^{bs}_{kl}\right) \quad (55)$$

$$X^{p,n+1}_{ij} = \frac{2}{3}(1-D^{n+1})C^{p}_{0}(1 + h_{C}\xi^{n+1})\alpha^{p,n+1}_{ij} \quad (56)$$

$$R^{p,n+1} = (1-D^{n+1})R^{p}_{\infty,0}(1 + h_{R}\xi^{n+1})r^{p,n+1} \quad (57)$$

$$Y^{E,n+1} = \frac{1}{2}\left(\epsilon^{n+1}_{ij} - \epsilon^{p,n+1}_{ij} - \xi^{n+1}\epsilon^{bs}_{ij}\right)E^{0}_{ijkl}\left(\epsilon^{n+1}_{kl} - \epsilon^{p,n+1}_{kl} - \xi^{n+1}\epsilon^{bs}_{kl}\right) \quad (58)$$

$$Y^{IN} = \frac{1}{3}C^{p}_{0}(1 + h_{C}\xi^{n+1})\alpha^{p,n+1}_{ij}\alpha^{p,n+1}_{ij} + \frac{1}{2}R^{p}_{\infty,0}(1 + h_{R}\xi^{n+1})(r^{p,n+1})^{2} \quad (59)$$

3.1. Elastic predictor – plastic corrector scheme

There is assumed that the total strain at the end of the time step, ϵ^{n+1}_{kl}, is known and defined as follows:

$$\epsilon^{n+1}_{kl} = \epsilon^{n}_{kl} + \Delta\epsilon_{kl} \quad (60)$$

Moreover, in the elastic – predictor step, the incremental strains are assumed to be elastic with no damage such that an initial trial stress can be computed as:

$$\sigma^{n+1,trial}_{ij} = (1-D^{n})E^{0}_{ijkl}\left(\epsilon^{n+1}_{kl} - \epsilon^{p,n}_{kl} - \xi^{n}\epsilon^{bs}_{kl}\right) \quad (61)$$

The trial state $\left(\sigma^{n+1,trial}_{ij}, \epsilon^{p,n}_{ij}, \alpha^{p,n}_{ij}, r^{p,n}, D^{n}, \xi^{n}\right)$ is used to check the yield criterion, Eq. 29.

If $f^{p,n+1\,trial}\left(\sigma^{n+1,trial}_{ij}\epsilon^{p,n}_{ij}\alpha^{p,n}_{ij}, r^{p,n}, D^{n}, \xi^{n}\right) \leq 0$ then $\sigma^{n+1}_{ij} = \sigma^{n+1,trial}_{ij}$ and the increment is completed.

Alternatively, if the yield function for trial stress is positive

$$f^{p,n+1\,trial}\left(\sigma^{n+1,trial}_{ij}\epsilon^{p,n}_{ij}\alpha^{p,n}_{ij}, r^{p,n}, D^{n}, \xi^{n}\right) > 0,$$

it means that current state lies outside of the yield surface. Plasticity has occurred and the state has to be returned to the yield surface. Thus, the system of equations from 49 to 54 is linearized and has to be solved with respect to the following unknowns

$$\mathbf{u} = \left\{\epsilon^{p,n+1}_{ij}, \alpha^{p,n+1}_{ij}, r^{p,n+1}, D^{n+1}, \xi^{n+1}, \Delta\lambda^{n+1}\right\}$$

with the initial condition

$$\epsilon^{p,n+1}_{ij} = \epsilon^{p,n}_{ij};\ \alpha^{p,n+1}_{ij} = \alpha^{p,n}_{ij};\ r^{p,n+1} = r^{p,n};$$

$$D^{n+1} = D^{n};\ \xi^{n+1} = \xi^{n};\ \Delta\lambda^{n+1} = 0;$$

The linearized system of six equations can be solved with the use of the Newton-Raphson scheme at iteration (s) what can be written in the following general form

$$\{\mathbf{R}\}^{s}_{n+1} + \left[\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}}\right]^{s}_{n+1}\{\delta\boldsymbol{u}\}_{n+1} + \cdots = \{\mathbf{0}\} \quad (62)$$

where, $\{\mathbf{R}\}^{T} = \{R^{\epsilon}_{ij}, R^{\alpha}_{ij}, R^{r}, R^{D}, R^{\xi}, R^{f}\}^{T}$, $[\partial\mathbf{R}/\partial\mathbf{u}]$ is the Jacobian defined as:

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{u}}\right] = \begin{bmatrix} \frac{\partial R^{\epsilon}_{ij}}{\partial \epsilon^{p,n+1}_{kl}} & \frac{\partial R^{\epsilon}_{ij}}{\partial \alpha^{p,n+1}_{kl}} & \frac{\partial R^{\epsilon}_{ij}}{\partial r^{p,n+1}} & \frac{\partial R^{\epsilon}_{ij}}{\partial D^{n+1}} & \frac{\partial R^{\epsilon}_{ij}}{\partial \xi^{n+1}} & \frac{\partial R^{\epsilon}_{ij}}{\partial \Delta\lambda^{n+1}} \\ \frac{\partial R^{\alpha}_{ij}}{\partial \epsilon^{p,n+1}_{kl}} & \frac{\partial R^{\alpha}_{ij}}{\partial \alpha^{p,n+1}_{kl}} & \frac{\partial R^{\alpha}_{ij}}{\partial r^{p,n+1}} & \frac{\partial R^{\alpha}_{ij}}{\partial D^{n+1}} & \frac{\partial R^{\alpha}_{ij}}{\partial \xi^{n+1}} & \frac{\partial R^{\alpha}_{ij}}{\partial \Delta\lambda^{n+1}} \\ \frac{\partial R^{r}}{\partial \epsilon^{p,n+1}_{kl}} & \frac{\partial R^{r}}{\partial \alpha^{p,n+1}_{kl}} & \frac{\partial R^{r}}{\partial r^{p,n+1}} & \frac{\partial R^{r}}{\partial D^{n+1}} & \frac{\partial R^{r}}{\partial \xi^{n+1}} & \frac{\partial R^{r}}{\partial \Delta\lambda^{n+1}} \\ \frac{\partial R^{D}}{\partial \epsilon^{p,n+1}_{kl}} & \frac{\partial R^{D}}{\partial \alpha^{p,n+1}_{kl}} & \frac{\partial R^{D}}{\partial r^{p,n+1}} & \frac{\partial R^{D}}{\partial D^{n+1}} & \frac{\partial R^{D}}{\partial \xi^{n+1}} & \frac{\partial R^{D}}{\partial \Delta\lambda^{n+1}} \\ \frac{\partial R^{\xi}}{\partial \epsilon^{p,n+1}_{kl}} & \frac{\partial R^{\xi}}{\partial \alpha^{p,n+1}_{kl}} & \frac{\partial R^{\xi}}{\partial r^{p,n+1}} & \frac{\partial R^{\xi}}{\partial D^{n+1}} & \frac{\partial R^{\xi}}{\partial \xi^{n+1}} & \frac{\partial R^{\xi}}{\partial \Delta\lambda^{n+1}} \\ \frac{\partial R^{f}}{\partial \epsilon^{p,n+1}_{kl}} & \frac{\partial R^{f}}{\partial \alpha^{p,n+1}_{kl}} & \frac{\partial R^{f}}{\partial r^{p,n+1}} & \frac{\partial R^{f}}{\partial D^{n+1}} & \frac{\partial R^{f}}{\partial \xi^{n+1}} & \frac{\partial R^{f}}{\partial \Delta\lambda^{n+1}} \end{bmatrix}$$

Solving the general equation Eq. 62 allows to obtain the corrections $\{\delta\mathbf{u}\}^{T} = \left\{\delta\epsilon^{p,n+1}_{ij}, \delta\alpha^{p,n+1}_{ij}, \delta r^{p,n+1}, \delta D^{n+1}, \delta\xi^{n+1}, \delta\Delta\lambda^{n+1}\right\}^{T}$ for the current iteration. Accordingly, the values of the unknowns for the next iteration are deduced from:

$$\left(\epsilon^{p,n+1}_{ij}\right)^{s+1} = \left(\epsilon^{p,n+1}_{ij}\right)^{s} + \delta\epsilon^{p,n+1}_{ij}$$

$$\left(\alpha^{p,n+1}_{ij}\right)^{s+1} = \left(\alpha^{p,n+1}_{ij}\right)^{s} + \delta\alpha^{p,n+1}_{ij}$$

$$(r^{p,n+1})^{s+1} = (r^{p,n+1})^{s} + \delta r^{p,n+1}$$

$$(D^{n+1})^{s+1} = (D^{n+1})^{s} + \delta D^{n+1}$$

$$(\xi^{n+1})^{s+1} = (\xi^{n+1})^{s} + \delta\xi^{n+1}$$

$$(\Delta\lambda^{n+1})^{s+1} = (\Delta\lambda^{n+1})^{s} + \delta\Delta\lambda^{n+1}$$

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The iteration proceeds until convergence is achieved based on an appropriate criterion of type $\{R\}_{n+1}^{s} < ERROR$.

Obtaining final values of unknowns the values of stress – like variables can be easily calculated by using the equations 55-59.

4. VALIDATION OF THE MODEL

The constitutive model of coupled phenomena has been validated by means of loading/unloading test performed at the temperature of liquid helium (4.2 K) (Egner and Skoczeń, 2010, Egner et al., 2015a). The experimental stress-strain curve for 316L stainless steel subjected to uniaxial tension is shown in Fig. 3. The evolution of micro-damage was measured by introducing unloading procedure and tracing variations of the unloading modulus. Parameters included in the evolution equations for thermodynamic forces (isotropic/kinematic hardening laws) and kinetic laws of evolution of internal variables (damage and phase evolution equations) were found with the use of ISIGHT program.

Accounting for three dissipative phenomena: plasticity, damage evolution 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 the temperature of 4.2K (see Fig. 3). Hardening effect due to phase transformation combined with softening effect due to damage evolution enables to model the initially nonlinear plastic hardening, followed by plastic plateau and strong nonlinear hardening in the final stage of plastic flow.

To show influence of the particular dissipative phenomena (damage evolution and phase transformation) on the model, three cases are presented (see Fig. 3): (a) only softening effect of damage was accounted for (no phase transformation); (b) only hardening effect of phase transformation was considered (damage development was neglected) and (c) both effects of damage evolution and phase transformation are included.

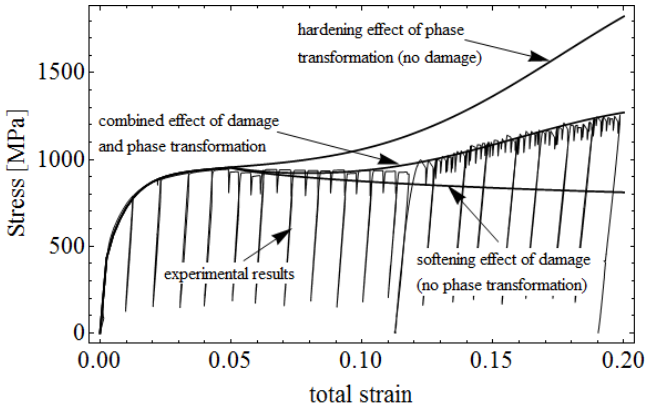

Fig. 3. Stress-strain curve for 316L stainless steel

The use of Bonora's law of damage evolution and Santacreu's kinetic model of phase transformation allows to obtain a very good agreement of the numerical results with experimental data (see Fig. 4). As was mentioned before, the use of total energy equivalence priciple imply that the damage energy release rate contains two terms: Y^E is the (classical) contribution of elastic energy and Y^{IN} represents the release of the stored energy due to the damage growth (Saanouni, 1994). It is worth to point it out that for some materials Y^{IN} represents more than 50% of the overall Y (Saanouni, 1988; Ju, 1989). The significant influence of Y^{IN} on damage evolution can be observed in Fig. 4 where using only classical term Y^E ($Y = Y^E$) in Eq. 37 caused about 50% drop of damage content in the RVE. The contribution of particular terms (Y^E and Y^{IN}) in Y is shown in Fig. 5.

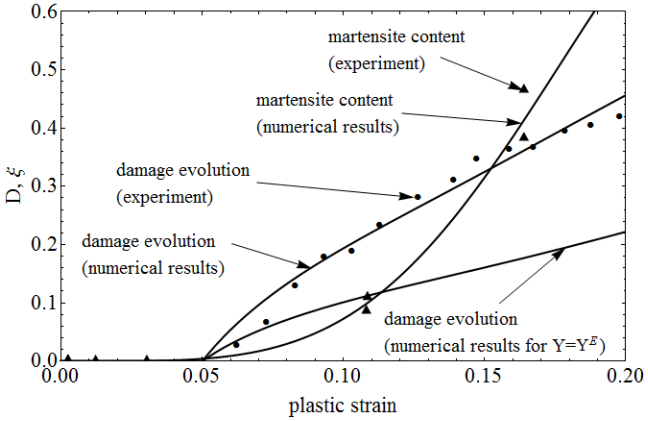

Fig. 4. Numerical and experimental results of damage evolution and martensite content versus plastic strain

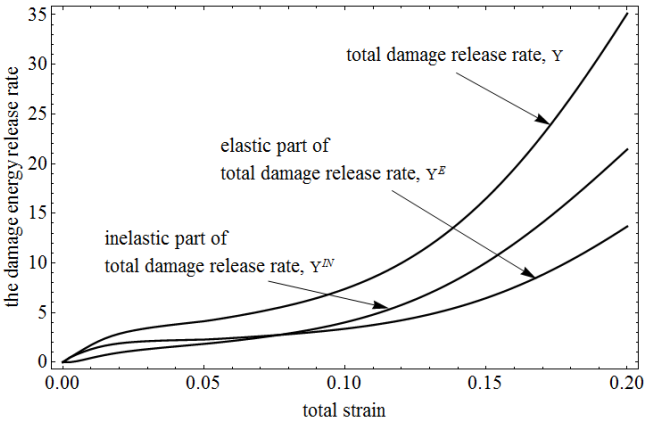

Fig. 5. The contribution of terms: Y^E and Y^{IN} in the total damage energy release rate Y

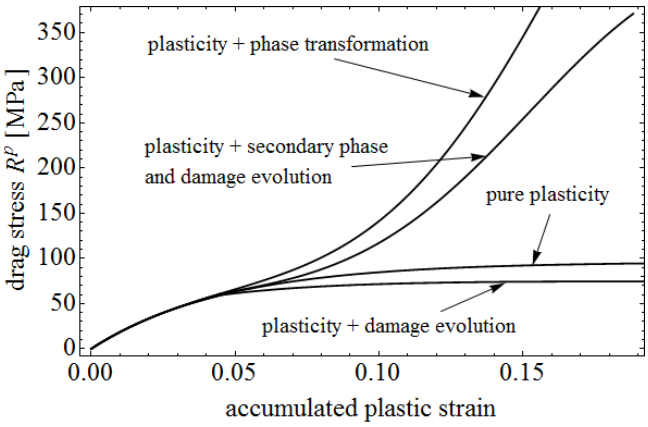

Fig. 6. Evolution of the drag stress

To examine the influence of the damage evolution and secondary phase content in the RVE on the isotropic (drag stress) and kinematic hardening (back stress) four cases are presented

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in Fig. 6 and Fig. 7: (a) pure plasticity (neither damge evolution nor phase transformation is present); (b) plasticity and the damage evolutios were accounted for (no phase transformation); (c) only hardening effect of phase transformation was considered (damage development was neglected) and (d) both effects of damage evolution and phase transformation are included. The use of the total energy equivalnce principle allowed to obtain full coupling between damge evolution and plastic flow, meaningfully the damage content effects the plastic modulus (see Eq. 23 and 24) and the drop of force – like varibles due to damage can be observed (Fig. 6 and Fig. 7). The use of simple linear function Eq. 47 and 48 also allowed to take into account important phenomenon like the strong influence of seconadary phase content on the hardening process (see Fig. 6 and Fig 7).

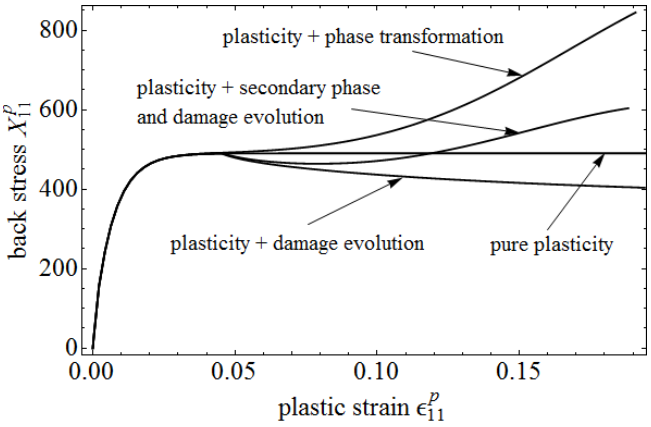

Fig. 7. Evolution of the back stress

Tab. 1. Material data for 316L stainless steel at the temperature of 4.2K

Young modulus [GPa]	206
Poisson ratio	0.3
Yield stress [MPa]	402.417
C_0^p [MPa]	82041.7
γ [MPa]	167
$R_{\infty,0}^p$ [MPa]	2104.24
b	22
h_C	1.03
h_R	7.3
Δv	0.02
D_0	0
D_C	0.8
α	200
n	4.5
S [MPa]	48.87
ξ^{max}	0.9
m	3.9
A	5.55

5. CONCLUSIONS

The constitutive model presented in the paper results from identification of two fundamental phenomena that occur in materials characterized by low stacking fault energy: plastic strain induced phase transformation and evolution of micro-damage reflected by decreasing elasticity modulus in the course of deformation. Non-associated theory was applied what allowed to obtain nonlinear isotropic and kinematic hardening. The influence of martensitic transformation on hardening process was modeled by introducing plastic moduli as functions of martensite content in the hardening laws. The total energy equivalence hypothesis is used to define the effective state variables. This approach enables: (1) the definition of internal state variables as well as the effective thermodynamic conjugated forces, which can be indifferently used in stress space and strain space by the use of the Legendre-Fenchel transformation; (2) obtaining symmetric physical properties of material (symmetric stiffness tensor, compliance tensor, strain hardening modules) even in the case of anisotropy induced by dissipative phenomena; (3) modeling of coupling between damage variable and other internal state variables in a natural way (Saanouni et. al., 1994). The average content of damage in the RVE (representative volume element) is described by one single scalar parameter. As was mentioned, this simplification is strong because martensitic phase is hard and behaves rather like rock-like material. Moreover, in brittle phases the stress state has the crucial influence on damage and anisotropic behavior of the material may take place. Thus, in the future work two separate scalar or tensorial type damage variable should be used (e.g. Kintzel et. al., 2010; Egner et. al., 2015).The model was validated through uniaxial tension test of 316L stainless steel, and a good agreement between the experimental and numerical results was obtained.

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