Modeling of Strain Localization and Failure in Vanadium under Quasistatic Loading

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Abstract The process of plastic deformation and failure of metals is accompanied by set of phenomena which cannot be easily modeled in the framework of classical models. The effects of strain localization and energy dissipation under deformation and failure require an adequate description of structure evolution at different stages of deformation process. This description can be developed based on the results of statistical model of typical mesodefect ensemble proposed in the Institute of continuous media mechanics UB RAS. The model takes into account bulk and shear parts of defect density tensor. Defect evolution is described by kinetic equations for two structural parameters: second order defect density tensor and scalar parameter, depending on the ratio of two characteristic scales (the mean size of defects and mean distance between them). The numerical simulation of strain localization and crack propagation were carried out in the finite-element package Simulia Abaqus Student Edition using procedure UMAT and XFEM.

Keywords defect evolution, energy dissipation, numerical simulation

1. Introduction

Nowadays investigation of metal fracture and knowledge of its laws have great importance in the developments of various designs and constructions. To create new technologies and improve existing ones one has to reach a more deep understanding of physical nature of failure. This understanding is needed in order to describe such phenomena, accompanying failure, as energy dissipation and strain localization.

Most existing models assume that the material failure takes place at the final stage of plastic deformation. However, the data obtained from systematic studies of defects evolution, carried out at Physical-technical institute named after A.F. Ioffe RAS [1] shows that the defects play the important role in deformation process at every stage of plastic deformation. These defects emergence at the early stage of deformation and effect on the microplasticity and failure processes. The models described the interaction between damage accumulation and plasticity processes were developed in [2-3] In this paper, the metal deformation behavior under quasi-static loading is described by one of such models, developed at the Institute of continuous media mechanics UB RAS.

The description of damage accumulation includes a consideration of the mesodefect ensemble evolution, their coherent development and interaction, the effect on the relaxation properties of materials and merging into the main crack.

The practical application of developed model requires both the verification of materials functions and generalization of the model for three dimension case. The most effective way for modeling of complex deformation phenomena is incorporation of this model for the standard finite - element packages.

This work is devoted to the generalization of developed earlier statistical based phenomenological elasto-visco-plastic model of defect evolution under deformation and failure in metals. The model takes into account defect density tensor separation bulk and shear parts. Defect evolution is described based on the kinetics of two parameters: the first parameter is second order defect density tensor, the second one - scalar parameter, depending on the ratio of two characteristic scales (the mean size of defects and mean distance between them).

The numerical simulation of strain localization on (plastic wave propagation) and crack propagation in plate vanadium specimen under quasi-static tension, compression of inclined cylindrical specimen were carried out in the finite-element package Simulia Abaqus using procedure UMAT. The big attention was paid on the calculation of plastic work and heat dissipation under investigated process. The results were compared with original experimental data, and with the results obtained using standard (incorporated in Abaqus) elasto–plastic model.

2. Mathematical model

Mesoscopic defects (mesoshears) can be described by the following tensor [3]

$$\mathbf{s}=\frac{1}{2}S\;\;\mathbf{lb}+\mathbf{bl}\;\;, \tag{1}$$

where $\mathbf{l}$- a unit normal to the shear plane, $\mathbf{b}$ - unit vector in the shear direction, S - shift intensity.

Averaging $\mathbf{s}$ over an elementary volume allows us to introduce the tensor parameter $\mathbf{p}$, which can be considered as a deformation caused by the defects:

$$\mathbf{p}=n\langle\mathbf{s}\rangle, \tag{2}$$

where n - defect density.

Application of dimension analysis allowed us to allocate the scale invariant structural parameter δ as

$$\delta=\left(\frac{L_n}{L_c}\right)^3, \tag{3}$$

where L_n - the mean size of the defect, L_c - the mean distance between the defects.

Solution of the self-consistency equation between the tensor micro- and macroparameters $\mathbf{s}$ and $\mathbf{p}$ allows us to establish three characteristic mode of δ [2,3]. For values of $\delta>\delta_*=1.3$, dependence of $p(\sigma)$ (the case of uniaxial loading) is monotone and the reaction of defect formation is reversible (Fig.1). There is a metastability respect to the parameter p, associated with the orientational degrees of mesoshears freedom in the range of $1\approx\delta_c<\delta<\delta_*$. For $\delta<\delta_c$ the jump of p becomes infinite; this characterizes unstable reaction of solid on the microshear formation.

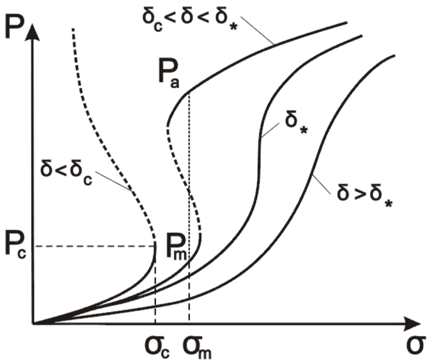

Figure 1. Typical response of a material on the defect growth

Material susceptibility to the defect growth in the deformation process in terms of δ should be determined by the current values of the structural scale i.e. the values of δ. It is also shown that these scales are determined by non-linear kinetics of $\mathbf{p}$ and thus, the defect density distribution determines the structural sensitivity to its further growth. The growth of the scales L_c, L_n means original structure "coarsening" and the general trend is decrease of δ, this allows to assume that plasticity mechanisms and the transition to failure are the sequential structure-scaling transitions in ensembles developing substructure defects.

Full strain rate can be represented as the sum of three components: elastic strain rate $\dot{\boldsymbol{\varepsilon}}^e$, plastic strain rate $\dot{\boldsymbol{\varepsilon}}^p$ and strain rate caused by defects:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p + \dot{\mathbf{p}} . \tag{4}$$

Elastic strains defined by linear Hooke's law:

$$\dot{\sigma}_0 = K\dot{\varepsilon}_0^e , \tag{5}$$

$$\dot{\boldsymbol{\sigma}}' = 2G\dot{\boldsymbol{\varepsilon}}'^e , \tag{6}$$

where K - isotropic elastic modulus, G - elastic shear modulus, σ_0 - spherical stress tensor, $\boldsymbol{\sigma}'$ - deviator of stress, ε_0 - spherical elastic strain tensor, $\boldsymbol{\varepsilon}'$ - deviator of elastic strain.

According to thermodynamic laws we can write dissipation inequality:

$$\boldsymbol{\sigma}' : \dot{\boldsymbol{\varepsilon}}^p - \frac{\partial F}{\partial \mathbf{p}} : \dot{\mathbf{p}} - \rho \mathbf{q} \cdot \frac{\nabla T}{T} \geq 0 , \tag{7}$$

where F is a part of the free energy, which is responsible for the energy defect subsystem, ρ - density, $\mathbf{q}$ - heat flux vector, T - temperature.

Assuming a qusilinear relationship between the thermodynamic forces and flows, there were obtained constitutive equations for calculating kinetics of plastic and structural strains:

$$\dot{\boldsymbol{\varepsilon}}^p = A_\sigma \boldsymbol{\sigma}' , \tag{8}$$

$$\dot{\mathbf{p}} = A_p \left(-\frac{\partial F}{\partial \mathbf{p}} \right) , \tag{9}$$

Parameters A_p, A_σ are kinetic coefficients having following form

$$A_\sigma = \exp\left(\frac{|\sigma|}{2G} \right) \frac{1}{2G\tau_\sigma} , \tag{10}$$

$$A_p = \exp\left(\frac{|\sigma|}{2G} \right) \frac{1}{2G\tau_p} . \tag{11}$$

These coefficients determine material relaxation properties due to the characteristic times of orientational transitions τ_p and relaxation transitions activated by stress τ_σ respectively. This form allows us to describe the aggregate of load curves at different strain rates.

Based on the received earlier the approximation of the non-equilibrium free energy (F) derivative of the $\mathbf{p}$ in one-dimensional case and on the assumption of coaxiality $\mathbf{p}$ and $\boldsymbol{\sigma}$, we can write

$$-\frac{\partial F}{\partial \mathbf{p}} = \frac{F_m}{p_c} \left[\frac{\boldsymbol{\Sigma}'}{\delta} + \frac{\boldsymbol{\gamma}}{\delta} - f(|\gamma|) \frac{\boldsymbol{\gamma}}{|\gamma|} - \boldsymbol{\gamma} \right] , \tag{12}$$

$$f(|\gamma|) = 0.0054 + \frac{0.5192(-0.0061 + 2|\gamma|)}{0.5814 - 0.0061|\gamma| + |\gamma|^2} , \tag{13}$$

where $\boldsymbol{\Sigma}' = \boldsymbol{\sigma}' / 2G$ - dimensionless stress deviator tensor, $\boldsymbol{\gamma} = \mathbf{p} / p_c$ - dimensionless deformation caused by defects, $p_c = \sqrt{\theta / \alpha}$, $F_m = \lambda\theta / \alpha^2$, θ - effective temperature factor responsible for the susceptibility of the system, $\alpha \sim G / V_0$, $V_0 \sim r_0^3$ - characteristic volume of the defect nucleus with radius r_0.

The system of equations (4)-(12) can be considered as a closed system of equation for modeling of damage accumulation and plasticity process in metals.

3. Numerical simulation

Numerical simulation was carried out using the finite element package Abaqus. Material behavior is described by a statistical – thermodynamic model introducing above using the procedure UMAT. Arrays of material constants, strain, strain increments and the time step passed as input data to the procedure. Increment of stress tensor components and increment of defect density tensor components are determined from the system of constitutive equations. Values of these components at the next time step are defined as the sum of values on the previous step and the appropriate increment.
There were considered numerical experiments on the quasi-static tensile of vanadium paddle, containing a central crack, compression of an oblique cylindrical vanadium sample and fracture of an oblique cylindrical titanium sample.
Quasi-static tensile experiment was carried out on the sample, the geometry of which is shown in Fig. 2. The specimen contains a central crack; its length is 3 mm.

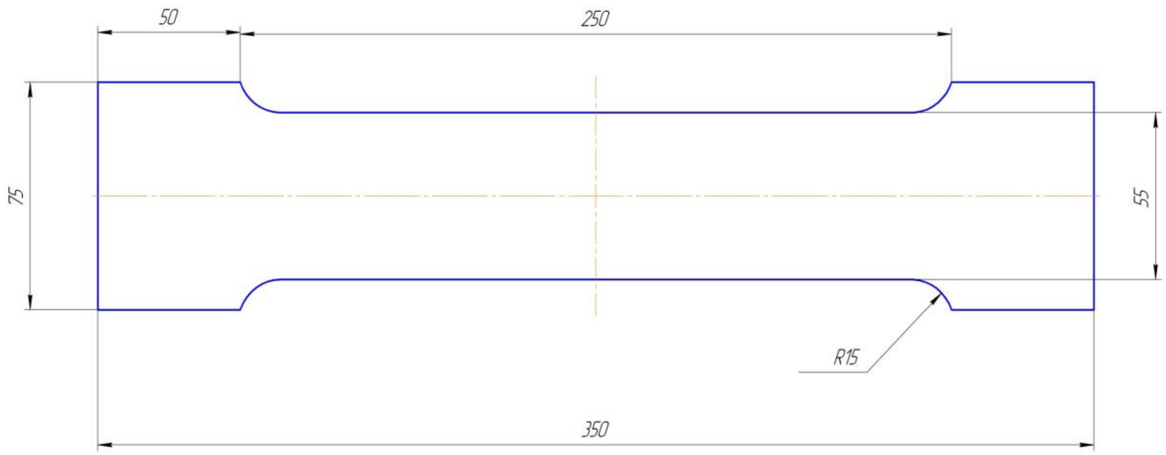

Figure 2. Geometry of specimen. All sizes are in millimeters.

The extended finite element method (XFEM) capability in Abaqus was used to model crack propagation. XFEM models a crack as an enriched feature by adding degrees of freedom in elements with special displacement functions. XFEM does not require the mesh to match the geometry of the discontinuities. It can be used to simulate initiation and propagation of a discrete crack along an arbitrary, solution – dependent path without the requirement of remeshing [5].
A maximum principal stress criterion was used to model the damage initiation. Stress state of the sample with a central crack after deformation is shown in Fig 3. Figure 4 displays the zoomed stress field near crack tip. The stress increases near the crack tip.

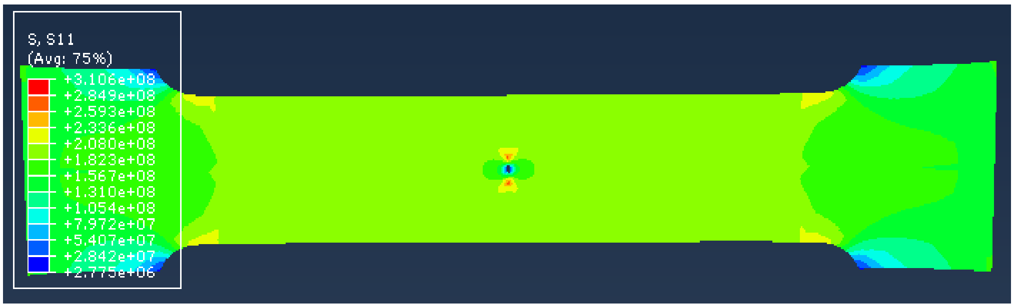

Figure 3. Component σ_{xx} (in the tension direction) of the stress tensor

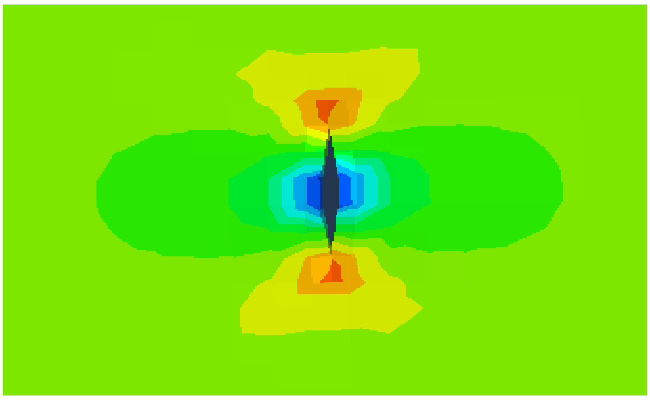

Figure 4. Stress distribution in the vicinity of the crack tip

Figures 5 shows deformation caused by defects area and figure 6 shows the shape of plastic zone. It can be seen that maximum strain localizes at the crack tip and gradually decreases with the distance from it. The magnitude of deformation, caused by defects is greater than the magnitude of plastic strain.

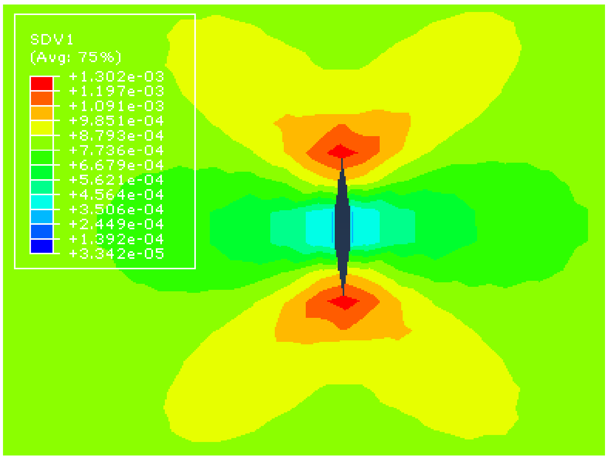

Figure 5. Component p_{xx} of the deformation tensor caused by defects near crack tip

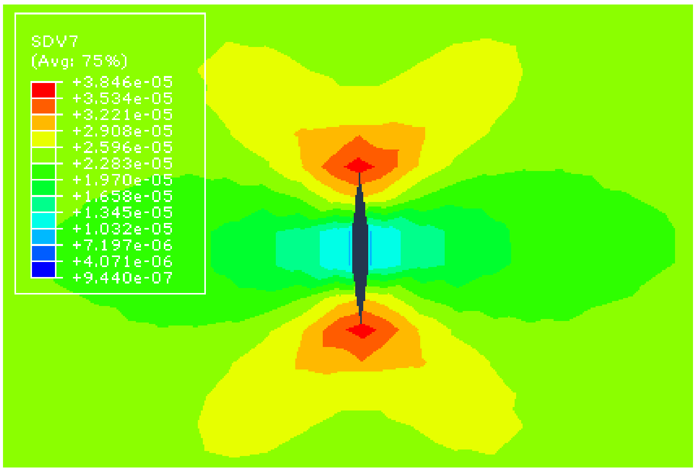

Figure 6. Component ε^{p}_{xx} of the plastic strain tensor near crack tip

Figures 7, 8 present the experimental temperature field on the specimen surface near crack tip and experimental obtained neat power near crack tip, respectively.

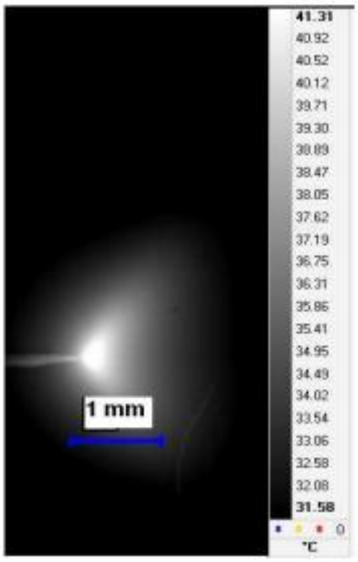

Figure 7. Experimental temperature field at the crack tip.

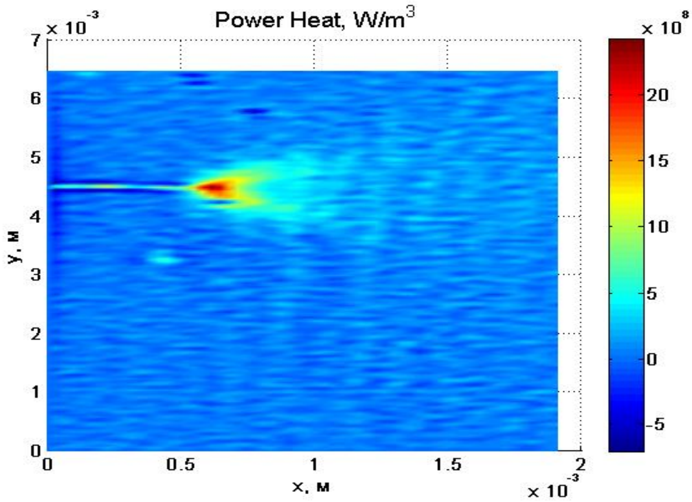

Figure 8. Experimental power of heat sources at the crack tip

Figure 9 demonstrates the strain energy distribution near crack tip. We can see several areas with the center at the crack tip and increasing radius, that is confirms the experimental data given above.

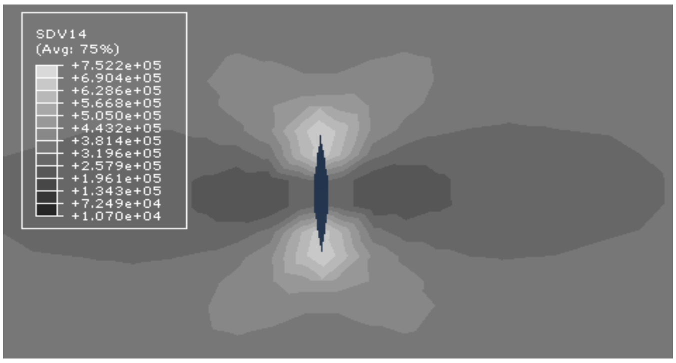

Figure 9. Numerical strain energy distribution near crack tip

Experiment on compression (Fig.10) was carried out with the vanadium samples. The specimen is an inclined cylinder; its diameter is 8 millimeters and its height is 4 millimeters. The cylinder was placed between the compressive planes; there was allowed its slip.

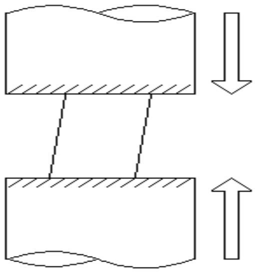

Figure 10. Experimental scheme on the quasi-static compression of vanadium

Figure 11 presents the stress-strain curves obtained experimentally (dashed line) and numerically (solid line). Results calculated by the described above model agree with experimental results.

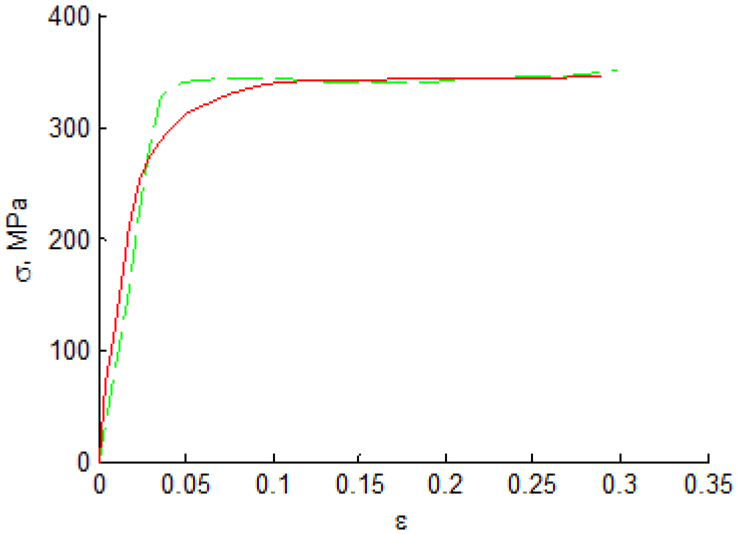

Figure 11. The simulation results of a cylindrical sample compression (dashed curve – the experimental results, the solid - numerical)

Figures 12 and 13 demonstrate various components of the plastic strain, and figures 14, 15 display the components of the deformation caused by defects. Red areas are zones where defect concentration is maximum. The experiment on the oblique sample compression was carried out to detect the shear bands in the sample, this can be seen in the simulation results. Figures 13 and 15 in cross section area show localization of these bands.

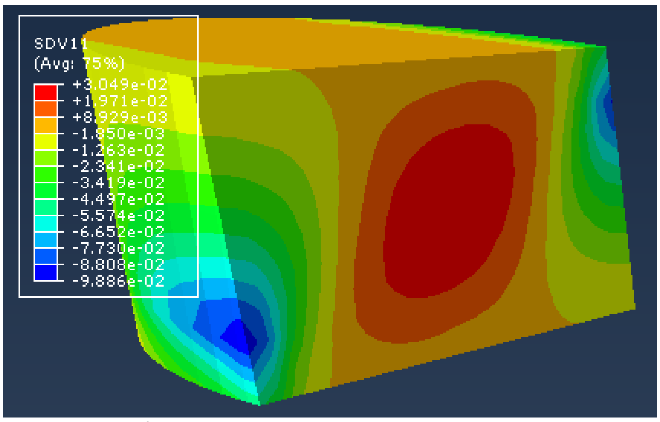

Figure 12. Component ε^{p}_{xz} of plastic strain tensor (cross section by the Oy plane)

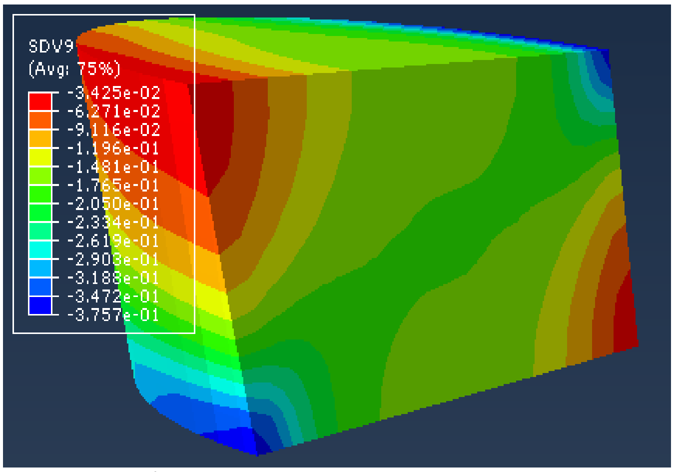

Figure 13. Component ε^{p}_{zz} of plastic strain tensor (cross section by the Oy plane)

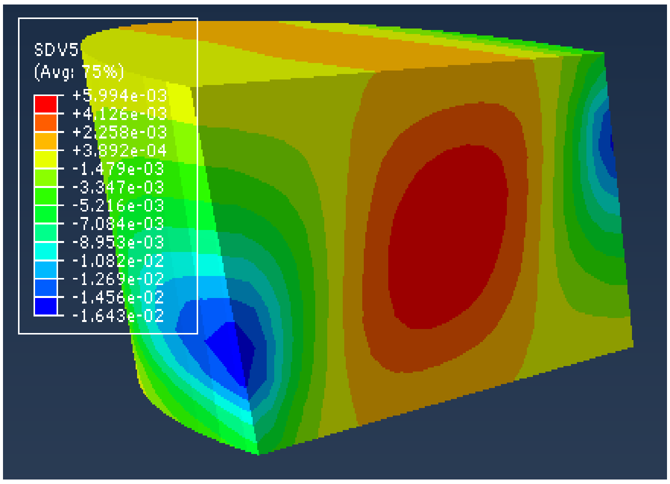

Figure 14. Component p_{xz} of the deformation tensor caused by defects

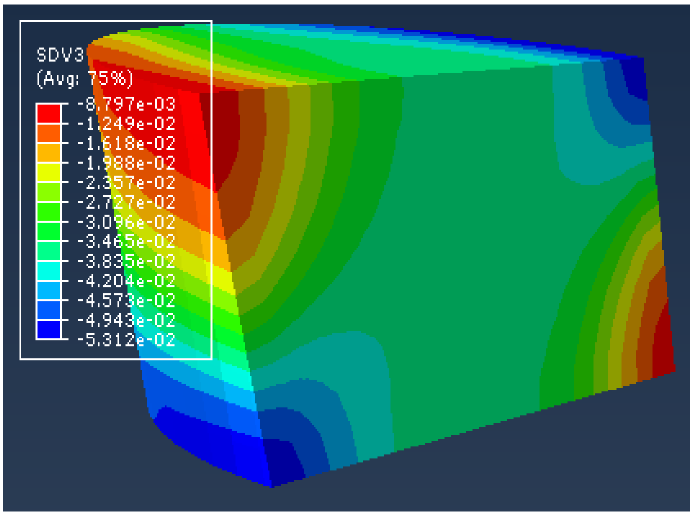

Figure 15. Component p_{zz} of the deformation tensor caused by defects

Also, there was carried out an experiment on the compression of titanium specimen of the same shape and the same sizes. The titanium with small grain size (about 0.3 mkm) is more brittle material then vanadium. The compression of this material is accompanied by crack initiation. Figure 16 presents a temperature distribution of the cracked specimen surface.

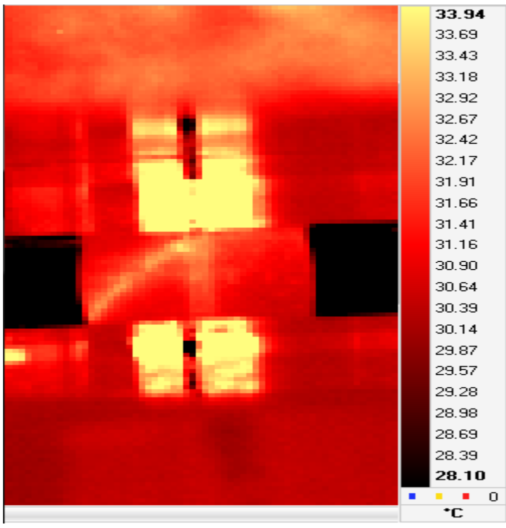

Figure 16. Cylindrical specimen after compression

Results of numerical modeling are shown in Figure 17. Maximum nominal shear stress criterion was used to initiate damage in cylinder sample. Crack location obtained by simulation is consistent with experimental data.

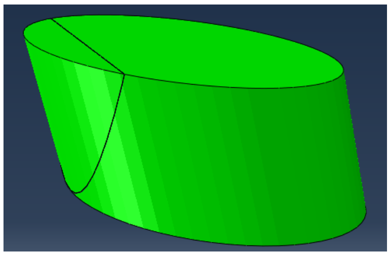
Figure 17. Numerical simulation results on the titanium specimen compression

3. Conclusion

The paper is devoted to the study of metal fracture processes under quasi-static loading. There were formulated constitutive equations for elasto-plastic medium with mesodefects. These equations were used for three-dimensional modeling of quasi-static vanadium paddle tension, compression of vanadium oblique cylinder and failure of titanium oblique cylinder sample. Numerical simulation was performed using finite-element package Abaqus by subroutine UMAT which allows user to implement his own constitutive equations. Fracture modeling was carried out using XFEM capability in Abaqus. Simulation results are in a good agreement with experimental data.

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