Ключові слова: ієрархія нелінійних рівнянь ББҐКІ, кінетичне рівняння, кореляційна функція, скейлінгова границя, активна м'яка речовина.

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SEVERE PLASTIC DEFORMATION BY KOBO METHOD – ESTIMATIONS AND MODEL

A new phenomenological model for the description and simulation of Severe Plastic Deformation (SPD) is developed based on the inverse dependence of the material's viscosity on the concentration of point defects (the higher the concentration, the less the viscosity). In this case, the local concentration of point defects is determined by (1) the intensity of deformation, (2) the annihilation of interstitial defects and vacancies, (3) the absorption of defects at dislocations, (4) diffusive redistribution of defects. The solution of the corresponding system of nonlinear differential equations for the field of defect concentrations and the differential equation for the velocity field at a given rate of deformation at the boundary of the sample provides a non-equilibrium phase transition - a jump in viscosity and a jump in the concentration of defects at a certain distance from the surface. In this case, the width of the zone of reduced viscosity and increased defect concentration is proportional to the surface velocity of the deformation. It is in this zone that it makes sense to consider the material as a viscous medium.

Keywords: severe plastic deformation, interstitial defects, vacancies, diffusion, viscosity, creep, nonlinear differential equations.

1. Introduction

An important example of nano-trend in science and technology during last decades is a production of nano-grained metals by Severe Plastic Deformation (SPD) [1, 2]. The most popular methods of SPD are ECAP (equi-channel angular pressing) and HPT (high-pressure torsion). Less than 20 years ago Korbel and Bochniak from AGH (Cracow) suggested their own method (KoBo) for extrusion of metals and alloys [3-5]. This method has something in common with HPT, but torsion is oscillating: the external surface is subjected to periodic rotations with a frequency of a few Hertz (say, 5 Hz) and amplitude of a few (6-8) degrees.

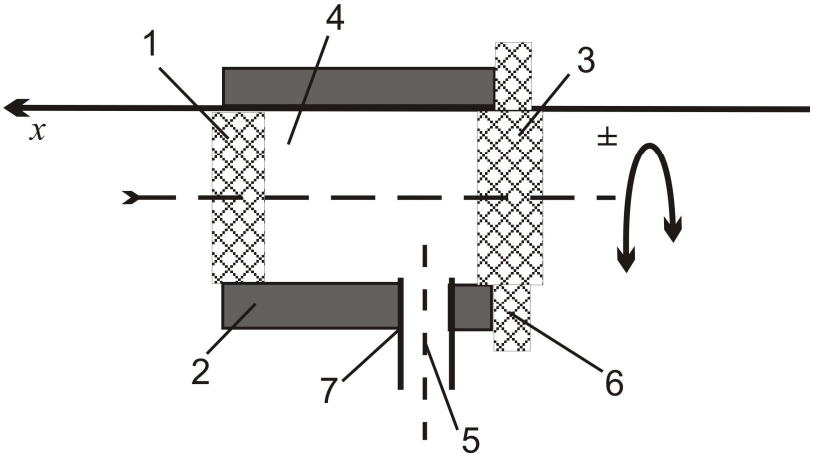

Figure 1. Scheme of KoBo lateral extrusion:
1—punch,
2—container,
3— reversibly rotating mandrel with ragging on the front surface,
4—extruded metal/billet,
5— product,
6—lock,
7— die located on container's side surface.

In the KoBo process, the metal billet undergoes reversible plastic twisting just before entering the cross section reducing die. The reversible metal twist does not affect directly the geometry of the billet, however, it transforms the typical for extrusion axio-radial flow into the layer like radial one. Experiments demonstrate that the metal flow during the KoBo process is actually a viscous flow, which follows Newton's law of laminar flow. They demonstrated that the metal within narrow layer around rotation zone becomes superplastic and is squeezed out practically as a viscous liquid with velocity about 0.5 mm/s. In addition, the measurements of the kinetics of metal flow have shown a linear dependence of extrusion stress on strain rate, i.e., the Newtonian type of the flow.

The first attempt of some elementary mathematical modeling of this process was made in [6], but it contained some artificial assumptions (like unknown non-zero viscosity in the non-deformed region, etc.). Here we try to construct some simple but self-consistent scheme for describing transition solid → viscous fluid due to the sharp increase of point defects concentrations under SPD.

2. Basic equations for creep, defect concentration and viscosity

According to the ideas of Korbel and Bochniak, we will assume that the main mechanism of KoBo process is based on interstitial defects and vacancies, generated by the interaction of dislocations in the process of oscillating intensive torsion. We will treat deformation in the active zone of the KoBo process as a creep generated by applied stress and provided by nonequilibrium defects generated by SPD. If creep is realized via bulk diffusion in the grains then we have Nabarro-Herring creep with deformation rate about

$$\frac{d\varepsilon}{dt} \approx \frac{D^{bulk}\Omega}{kT}\frac{1}{l^2}\sigma \qquad (1)$$

Here D^{bulk} is a self-diffusivity in the bulk of the grain, Ω is an atomic volume, kT is a Boltzmann constant times temperature, l is a mean grain size, σ is a local stress. Bulk diffusivity can be represented in terms of products of the interstitial and vacancy diffusivities D_i, D_V and respective defect concentrations (ratio of defects and atoms) $N_i, N_V : D^{bulk} \approx N_i D_i + N_V D_V$.

If creep is realized via grain-boundary diffusion then we have Coble creep with deformation rate about

$$\frac{d\varepsilon}{dt} \approx \frac{D^{GB}\Omega}{kT}\frac{\delta}{l^3}\sigma \qquad (2)$$

Here D^{GB} is a mean self-diffusivity within grain-boundary, δ is a width of grain boundary, typically from half to one nanometer. Typically, at equilibrium conditions at low temperatures and small grains, Coble creep is more realistic. Yet, in our case, when the nonequilibrium defect concentration is rather high in the bulk and bulk diffusivity may be not less than the grain-boundary one, we will treat Nabarro-Herring creep mode as the main one. Then we may treat the coefficient before stress on the right-hand side of Eq. (1) as inverse dynamic viscosity. Thus, in our simplified model, the viscosity will be estimated from the expression

$$\eta \approx \frac{kT}{\left(N_i D_i + N_V D_V\right)\Omega} l^2 \tag{3}$$

Here we neglect the turbulence effect, and the distribution of tangential velocities, initiated by external rotation, is given by simplified equation

$$\frac{\partial V_y(t,X)}{\partial t} = \frac{\partial}{\partial X}\left(\eta\left(N_i(t,X)N_V(t,X)\right)\frac{\partial V_y}{\partial X}\right) \tag{4}$$

Actually, we will work only with amplitudes of tangential velocities, therefore we will further treat V_y as the local amplitudes. Here we are interested in the steady-state regime of the KoBo process, when $\frac{\partial V_y}{\partial t} \approx 0$. Then

$$\eta\left(N_i(t,X)N_V(t,X)\right)\frac{\partial V_y}{\partial X} \approx const = -\sigma_{cr}, \tag{5}$$

here σ_{cr} is a strength limit, providing plastic deformation, movement, and annihilation of dislocations leading to the generation of point defects. Velocities amplitudes should, therefore, decrease from the maximum value $V_y(X=0) = V_{\max}$ at the rotating surface, in the X-direction:

$$V_y(X) = V_{\max} - \sigma_{cr}\int_0^X \frac{1}{\eta(X')}dX' \tag{6}$$

Naturally, at some point $X = H$ velocity will come to zero: $V_y(X=H) = 0 = V_{\max} - \sigma_{cr}\int_0^H \frac{dX}{\eta(X)}$. H has a physical meaning of the active zone width in the KoBo process. It is determined by the condition (integral equation):

$$\int_0^H \frac{dX}{\eta(X)} = \frac{V_{\max}}{\sigma_{cr}} \tag{7}$$

At X>H one may treat velocity as zero and viscosity as practically infinite (practically zero defect concentration).

To have the self-consistent description of KoBo process, one has to predict (at least roughly) the defect concentrations and the mean grain size in the active zone. For this, we should somehow describe the energy dissipation per unit volume of the active zone. It can be done by several methods.

The first method is almost school-like and based on the work of deformation:

Torsion force of the external source is about $M \approx F_{cr}R$, where R is a radius of the rotating part. (Here we neglect the factors like 1/2). Work per one oscillation is about $A_1 \approx M \cdot \varphi_{\max} \approx \left(\sigma_{cr}\pi R^2\right)\cdot R \cdot \varphi_{\max}$ with $\varphi_{\max}$ as an amplitude angle of rotation,

$\varphi_{\max} \approx V_{\max} / \nu / R$ (typically 6-8 degrees). Work per unit time is $\frac{dA}{dt} \approx \left(\sigma_{cr} \pi R^2\right) R \varphi_{\max} \nu$ with ν as a frequency of external rotations (typically a few times per second, say 5Hz). The volume of active zone is about $\pi R^2 H$. Thus, the energy dissipation per unit volume (w) is about

$$w \approx \frac{1}{\pi R^2 H}\left(\sigma_{cr} \pi R^2\right) R \varphi_{\max} \nu = \frac{\sigma_{cr} \varphi_{\max} R \nu}{H} \tag{8}$$

Second, the alternative way is to use the expression for energy dissipation in viscous media (Landau, [7]):

$$w = \eta \left(\frac{\partial V}{\partial X}\right)^2 \tag{9}$$

Using eq. (5) for the steady-state regime, one can reformulate eq. (9) as

$$w \approx \frac{\sigma_{cr}^2}{\eta} \approx \sigma_{cr} \frac{\partial V}{\partial X} \approx \sigma_{cr} \frac{V_{\max}}{H} \approx \sigma_{cr} \frac{\varphi_{\max} R \nu}{H} \tag{10}$$

As one can see, equations (8) and (10) give the same energy dissipation per unit volume.

Dissipation per atomic volume is

$$w\Omega \approx \frac{\sigma_{cr}^2}{\eta} \Omega \approx \sigma_{cr} \frac{\varphi_{\max} R \nu}{H} \Omega .$$

If one assumes that some fraction $\overline{\omega}_r$ of energy dissipation is used for generation of the interstitial defects (with E_i^{form} being a formation energy of interstitial defect), then the average number of interstitials generated per unit volume per unit time is

$$\overline{q}_i = r \frac{w}{E_i^{form}} \approx r \frac{\sigma_{cr}^2}{\eta E_i^{form}} \approx r \sigma_{cr} \frac{\varphi_{\max} R \nu}{H E_i^{form}} .$$

Then the generation of defects per unit atomic cell pet unit time is

$$\overline{q}_{i1} \approx r \sigma_{cr} \frac{\varphi_{\max} R \nu}{H E_i^{form}} \Omega \tag{11}$$

In our model, we admit the nonuniform distribution of defects and corresponding viscosity. Therefore, in general case we should use the following expression (without using H but using an expression for viscosity):

$$q_{i1} = \begin{cases} r \frac{\sigma_{cr}^2}{\eta E_i^{form}} \Omega \approx r \frac{\sigma_{cr}^2 \Omega^2}{l^2 kT E_i^{form}} \left(N_i D_i + N_V D_V\right), \; X < H \\ 0, X > H \end{cases} \tag{12}$$

(generation of defects proceeds only within the active zone).

We will further assume that the generation of vacancies proceeds simultaneously with interstitials (like in Frenkel pairs production), and will approximately assume $q_{i1} \approx q_{V1} \equiv q_1$.

Thus, we can now formulate the basic equations for the defect concentrations (mole fractions):

$$\frac{\partial N_i}{\partial t} = q_1 - \frac{N_i}{\tau_i} - \alpha D_i N_i N_V + D_i \frac{\partial^2 N_i}{\partial X^2} \tag{13}$$

$$\frac{\partial N_V}{\partial t} = q_1 - \frac{N_V}{\tau_V} - \alpha D_i N_i N_V + D_V \frac{\partial^2 N_V}{\partial X^2} \tag{14}$$

Here we did not take into account the flux of defects in the stress gradient. It is important for extrusion but not for the redistribution of defects (see below). Second terms on the right-hand side of eq. (13,14) are responsible for the sinks of interstitials and vacancies, mainly at the dislocations. The values $L_i = \sqrt{D_i \tau_i}, L_V = \sqrt{D_V \tau_V}$ are treated as the migration paths of interstitials and vacancies to the dislocations. The third term in both equations (13,14) is responsible for the annihilation of interstitials and vacancies, $\lambda = 1/\sqrt{\alpha}$ is a distance at which vacancies and interstitials start to "feel each other", $\lambda^2 / D_i = 1/(\alpha D_i)$ is a time for a couple to annihilate. Interstitial diffusivity D_i is used here since interstitials diffuse much faster than vacancies.

We are interested in the observable steady-state KoBo regime. Therefore, we will take the time derivatives of defects concentrations as zero:

$$q_1 - \frac{N_i}{\tau_i} - \alpha D_i N_i N_V + D_i \frac{\partial^2 N_i}{\partial X^2} \approx 0 \tag{15}$$

$$q_1 - \frac{N_V}{\tau_V} - \alpha D_i N_i N_V + D_V \frac{\partial^2 N_V}{\partial X^2} \approx 0 \tag{16}$$

Moreover, we will see below by direct calculations that the transient layer between active and inert zones is significantly less than the active zone with H. Therefore, we will start our evaluations from the points in active zone far from H, where both concentrations are almost constant:

$$q_1 - \frac{N_i}{\tau_i} - \alpha D_i N_i N_V \approx 0. \tag{15'}$$

$$q_1 - \frac{N_V}{\tau_V} - \alpha D_i N_i N_V \approx 0. \tag{16'}$$

Comparison of eqs. (15, 16) implies:

$$\frac{N_i}{\tau_i} = \frac{N_V}{\tau_V} \Rightarrow \frac{N_V}{N_i} = \frac{\tau_V}{\tau_i} = \frac{L_V^2}{L_i^2}\frac{D_i}{D_V} \tag{17}$$

If the sinks of vacancies and interstitials are the same dislocations then the migration lengths should be the same ($\frac{L_V^2}{L_i^2} = 1$) and

$$\frac{N_V}{N_i} = \frac{D_i}{D_V} \Leftrightarrow N_V D_V = N_i D_i \tag{18}$$

Of course eq. (18) is only an approximation, but we will use it below for our estimations. In particular, in this case the viscosity and defect source expressions (3,12) become following:

$$\eta \approx \frac{kTl^2}{2D_i\Omega}\frac{1}{N_i} \tag{19}$$

$$q_1 = \begin{cases} r\dfrac{2\sigma_{cr}^2\Omega^2}{l^2 kTE_i^{form}} D_i N_i, & X < H \\ 0, & X > H \end{cases} \tag{20}$$

Substituting eqs. (18, 20) into eq. (15) or (16), one gets approximate steady-state uniform (averaged) solution for the active zone X<H:

$$r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}}D_iN_i = D_i\frac{N_i}{L^2} + \alpha D_i\frac{D_i}{D_{V\,i}}N_i^2 \Rightarrow$$

$$N_i^{st} = \frac{D_V}{\alpha D_i}\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1}{L^2}\right) \quad \text{at X<H.} \tag{21}$$

Thus, physically realistic solution with high defect density is possible only under condition

$$r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} > \frac{1}{L^2} \tag{22}$$

Otherwise, the non-zero solution is possible only with diffusion term and will give the active zone only of the magnitude of defect migration path L which is not centimeters as in KoBo but microns.

Substituting Eq. (21) into Eq. (19), one can predict an average viscosity in the active zone of KoBo:

$$\eta \approx \frac{kTl^2\alpha}{2D_V\Omega}\frac{1}{\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1}{L^2}\right)_i} \tag{23}$$

Substituting rq. (23) into eq.(7),one can estimate the width H of an active zone:

$$H = \eta\frac{V_{\max}}{\sigma_{cr}} = \frac{kTl^2\alpha}{2D_V\sigma_{cr}\Omega}\frac{V_{\max}}{\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1}{L^2}\right)_i} \tag{24}$$

3. Estimations

We will use the following values of the main parameters, part of which are substantiated in our previous paper [6], but which earlier had been used for another model:

$r = 0.5, \sigma_{cr} = 10^8\,Pa,\ L = 10^{-6}m,\ l = 10^{-8}m,\ \Omega = 10^{-29}m^3,\ E_i^{form} = 10^{-18}J,$

$T = 300K, D_i = 10^{-5}m^2/s, D_i/D_V = 10^4,\ \alpha = 10^{18}m^{-2}$

Average defect concentration in the active zone:

$$N_i^{st} = \frac{D_V}{\alpha D_i}\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1}{L^2}\right) \approx 1.4\cdot 10^{-10},$$

$$N_V^{st} = \frac{D_i}{D_V}N_i^{st} \approx 1.4\cdot 10^{-6}$$

Average viscosity in the active zone:

$$\eta^{st} \approx \frac{kTl^2}{2D_i\Omega}\frac{1}{N_i^{st}} \approx 1.5\cdot 10^7\,Pa\cdot s$$

Maximal velocity of tangential motion:

$$V_{\max} \approx \varphi_{\max}R\nu \approx 0.1m/s$$

Approximate width of active KoBo zone:

$$H = \eta\frac{V_{\max}}{\sigma_{cr}} = \frac{kTl^2\alpha}{2D_V\sigma_{cr}\Omega}\frac{V_{\max}}{\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1}{L^2}\right)_i} \approx 1.5\cdot 10^{-2}m$$

Thus, we predict the active zone width about centimeter which is rather close to the real case.

4. Mathematical model including diffusive redistribution

Now we consider the non-uniform model including the diffusive redistribution of defects but preserving the steady-state approximation. In this case, two equations (15,16) are reduced to the following form:

$$\begin{cases} \left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1_i}{L_i^2} \right) N_i - \alpha\frac{D_i}{D_V}N_i^2 + \frac{\partial^2 N_i}{\partial X^2} \approx 0,\ X < H \\ \left(-\frac{1_i}{L_i^2} \right) N_i - \alpha\frac{D_i}{D_V}N_i^2 + \frac{\partial^2 N_i}{\partial X^2} \approx 0,\ X > H \\ N_V(X) = \frac{D_i}{D_V}N_i(X) \end{cases} \quad (25)$$

$$\eta(X) \approx \frac{kTl^2}{2D_i\Omega}\frac{1}{N_i(X)},\ \int_0^H \frac{dX}{\eta(X)} = \frac{V_{\max}}{\sigma_{cr}}.$$

To get the numeric solution, it is convenient to use the non-dimensional length $\xi = X/H,\ \Delta\xi = 1/M$. Then $H\int_0^1 \frac{d\xi}{\eta(\xi)} = \frac{V_{\max}}{\sigma_{cr}}$, so that

$$H = \frac{V_{\max}}{\sigma_{cr}\int_0^1 \frac{d\xi}{\eta(\xi)}} \quad (26)$$

Then we have the finite difference equation:

$$A[k]N_i[k] - B\left(N_i[k]\right)^2 + \frac{N_i[k-1] + N_i[k+1] - 2N_i[k]}{1/M^2} = 0$$

$$A[k] = \begin{cases} H^2\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}} - \frac{1}{L_i^2} \right),\ 1 < k < M-1 \\ \left(-\frac{H^2}{L_i^2} \right),\ M <= k < 2M \end{cases} \quad (27)$$

$$B = H^2\alpha\frac{D_i}{D_V}$$

To get the iteration scheme, we treat $N_i[k]$ in eq. (26) as a new iteration and $N_i[k-1]$, $N_i[k+1]$ as a previous iteration, so that one has the quadratic equation for the new iteration. Choosing (naturally) only the positive root, one obtains:

$$N_i^{new}[k] := \frac{M^2}{2B}\left(A[k]/M^2 - 2 + \sqrt{\left(2 - A[k]/M^2\right)^2 + 4B/M^2 \cdot \left(N_i[k-1] + N_i[k+1]\right)} \right), \quad (28)$$

$1 \le k \le 2M-1$

Boundary conditions are following:

$N_i[0] := N_i[1],\ N_i[2M] := N_i[2M-1]$.

After finding the next iteration for the defect concentration, we find the new iteration for the active zone width

$H^{new} := \frac{V_{\max} kTl^2}{\sigma_{cr} D_i \Omega \int_0^1 N_i(\xi) d\xi} = \frac{V_{\max} k_B Tl^2 M}{\sigma_{cr} D_i \Omega \sum_{k=0}^{M-1} N_i^{new}[k]}$. Zero iteration is taken from homogeneous approximation without diffusion: for defect concentration eq. (21) for k<M and zero for k>m, and for H-equation (24).

Calculations demonstrate that our iteration scheme converges very fast and effectively.

5. Numerical results

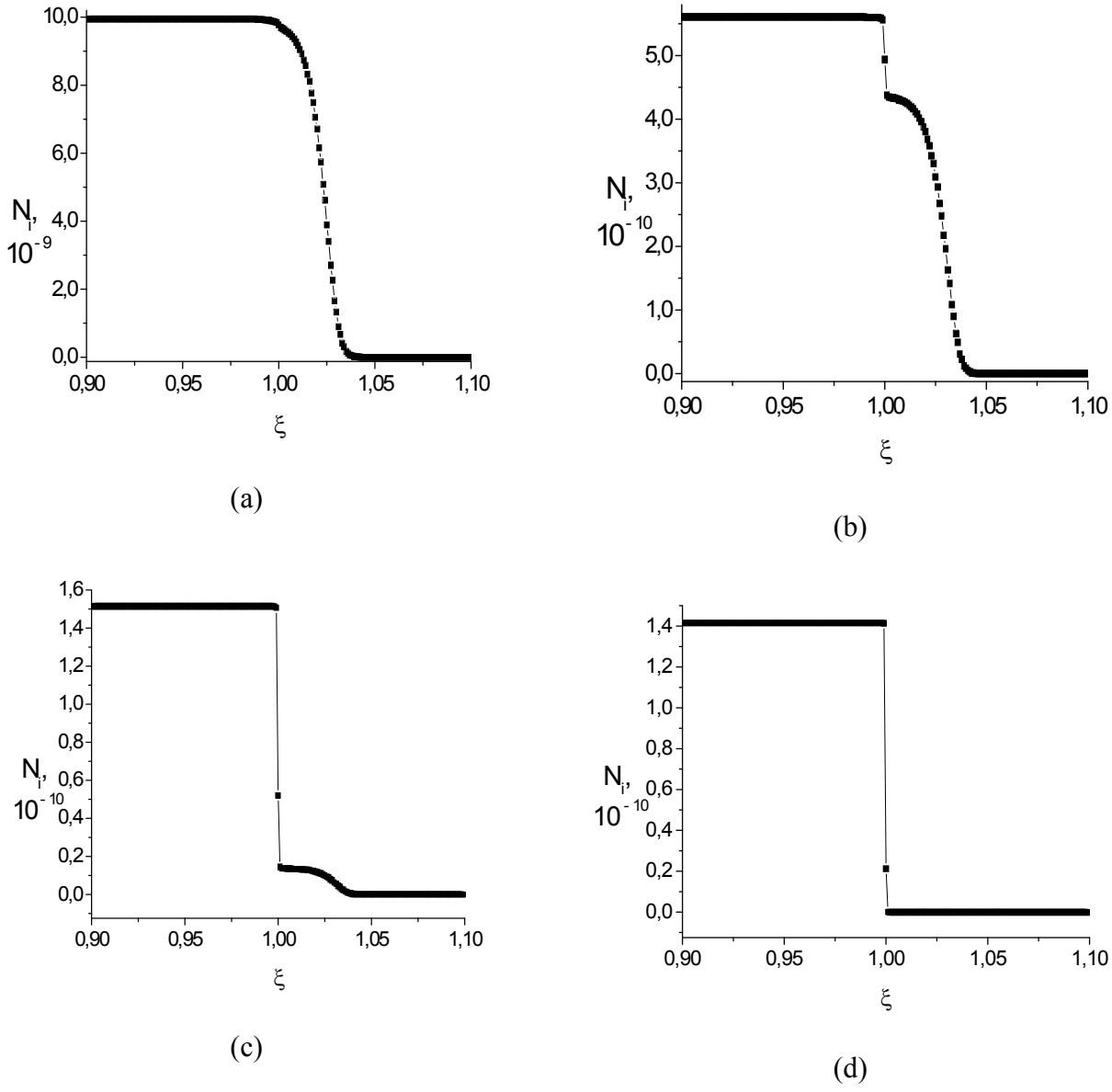

Figure 2. Convergence of concentration profile for interstitials according to iteration procedure eq. 28 after 80 (a), 82 (b), 83 (c), 91 (d) iterations.

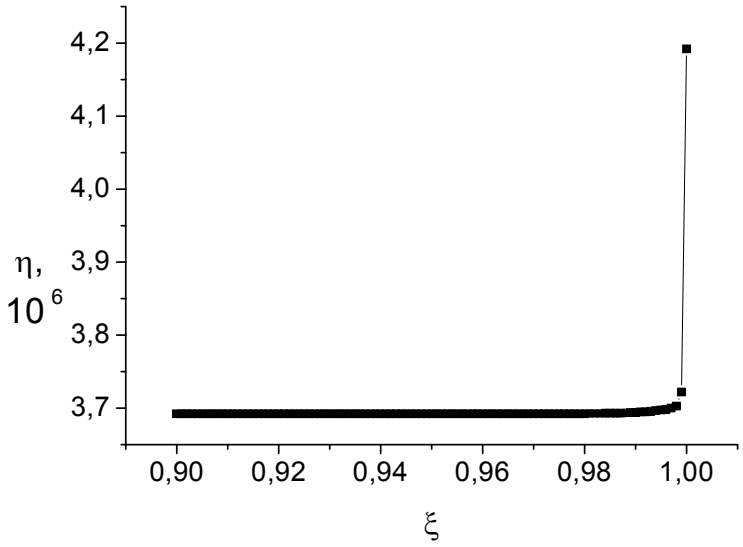

Figure 3. Non-equilibrium phase transition under KoBo-process – sharp decrease of viscosity within active deformation zone ($0< x < H$, $H \approx \frac{kTl^2\alpha}{2D_V\sigma_{cr}\Omega}\frac{V_{\max}}{\left(r\frac{2\sigma_{cr}^2\Omega^2}{l^2kTE_i^{form}}-\frac{1}{L^2}\right)}$)

5. Conclusions

1. New phenomenological scheme of SPD description for KoBo method of extrusion is developed. Viscosity is treated in terms of Nabarro-Herring creep under high concentration of defects generated by external oscillating rotations at the surface of the sample.
2. Generation of defects is estimated in the terms of energy dissipation in viscous media.
3. Non-equilibrium phase transition solid→viscous is described.
4. The width of active zone and defect concentration in active zone is predicted.
5. Account of diffusive redistribution of defects changes results insignificantly.

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Анотація. ***А.М. Гусак, А.Р. Гонда. Інтенсивна пластична деформація КоВо-методу – оцінки та модель.*** *Розвинута нова, феноменологічна концепція опису та моделювання інтенсивної пластичної деформації (ІПД), основана на оберненій залежності в'язкості матеріалу від концентрації точкових дефектів (чим більше ця концентрація, тим менше в'язкість). При цьому локальна концентрація точкових дефектів визначається, (1) інтенсивністю деформації, (2) анігіляцією міжвузлових дефектів та вакансій, (3) поглинанням дефектів на дислокаціях, (4) дифузійним перерозподілом дефектів. Розв'язок відповідної системи нелінійних диференціальних рівнянь для поля концентрацій дефектів та диференціального рівняння для поля швидкостей при заданій швидкості деформації на границі зразка дає нерівноважний фазовий перехід – стрибок в'язкості і стрибок концентрації дефектів на певній відстані від поверхні. При цьому ширина зони пониженої в'язкості та підвищеної концентрації дефектів пропорційна поверхневій швидкості деформації. Саме в цій зоні має сенс розглядати матеріал як в'язке середовище.*

Ключові слова: інтенсивна пластична деформація, міжвузлові дефекти, вакансії, дифузія, в'язкість, повзучість, нелінійні диференціальні рівняння.

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