Modeling of Metal Strengthening During Severe Plastic Deformation

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Abstract

The theory of nonequilibrium evolutionary thermodynamics (NET) is applied [1, 2]. Changes in internal energy are represented in the form of a thermodynamic identity, which includes the law of energy conservation, taking into account energy exchange with the external environment and its transformation at the level of internal degrees of freedom during relaxation. Therefore, within the studied method, we considered processes where energy is replenished through the work of external sources of heat and relaxation processes. The relaxation of the system occurs in two ways: on the one hand, through an increase in the number of structural defects, and on the other, through the production of heat (formation of entropy). The study showed that at the initial stage of the process of energy increase, the growth of internal energy dominates due to the intensification of defects. This growth occurs due to the increase in the number and average energy of defects.

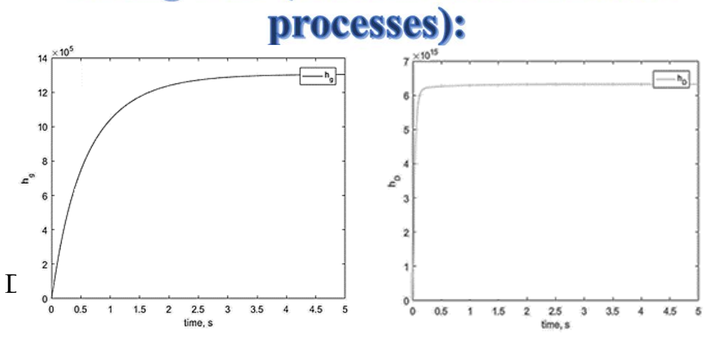
In the study, methods for the production of nanostructured materials were also analysed, in particular, methods of severe plastic deformation and approaches of nonequilibrium evolutionary thermodynamics. We consider a model of two-defect approximation, key relations in the context of internal energy and the phasing of the fragmentation process. We investigate how the densities of dislocations and grain boundaries change over time and also analyse these changes taking into account nonlinear connections. As an example, we show that the density of dislocations transforms from lower to significantly higher levels at the beginning of severe plastic deformation, indicating a structural phase transition. After that, although dislocations stabilize at a steady level, the density of grain boundaries continues to grow and reaches a steady value more slowly, following the dynamics of dislocation density.

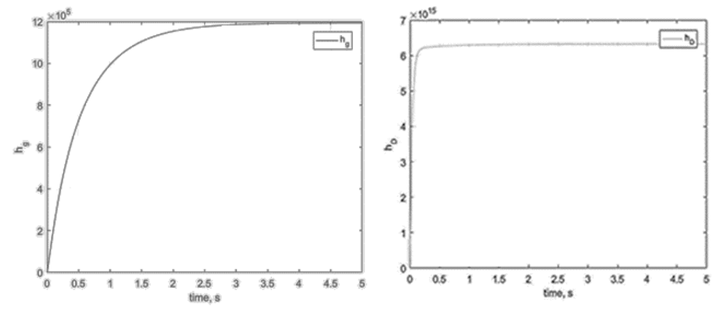
The study outlines how external stresses depend on the density of grain boundaries, taking into account nonlinear connections. It has been found that this dependence is generally represented by a monotonically decreasing curve, which does not show pronounced jumps or fluctuations. A change in the slope of the curve can be noticed in the zone of structural phase transition, which can significantly affect the change in the material strengthening law.

Problem statement

Within the framework of noequilibrium evolutionary thermodynamics, we investigate the process of fragmentation of a metal structure under severe plastic deformation (SPD). Analyze the time dependencies of dislocation densities and grain boundaries and the influence of the latter on the behavior of external stresses and elastic strains. Modify the software suite for obtaining research results and also construct the laws of strengthening.

Patterns of defect formation during DIP (deformation-induced processes):

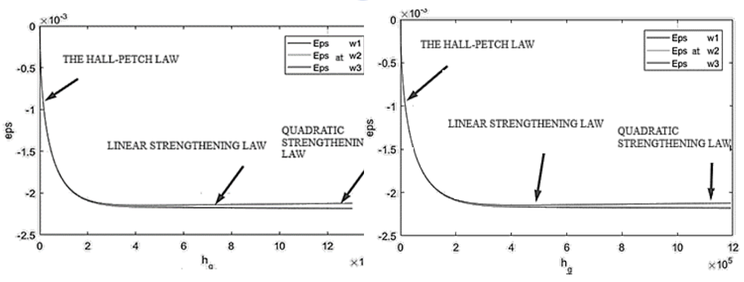




Defect kinetics $h_g(t)$ with a nonlinear relationship.

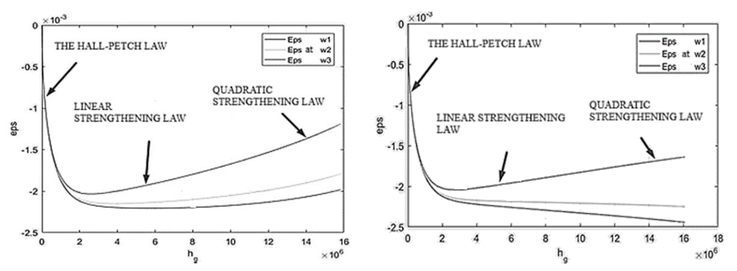
Defect kinetics $h_D(t)$ with a nonlinear relationship.

Hardening curves



Hardening curves, including the influence of grain boundary (GB) sliding:
$w_1 = 0$, $w_2 = 1{,}2 \times 10^{-11}$, $w_3 = 5 \times 10^{-11}$.

Hardening curves with a nonlinear relationship, including the influence of grain boundary (GB) sliding
$w_1 = 0$, $w_2 = 1{,}2 \times 10^{-11}$, $w_3 = 5 \times 10^{-11}$.



Hardening curves, including the influence of grain boundary (GB) sliding:
$w_1 = 0$, $w_2 = 1{,}2 \times 10^{-11}$, $w_3 = 5 \times 10^{-11}$
and with an increase in the parameter φ_{0g} by 50 times.

Hardening curves with a nonlinear relationship, including the influence of grain boundary (GB) sliding: $w_1 = 0$, $w_2 = 1{,}2 \times 10^{-11}$, $w_3 = 5 \times 10^{-11}$
and with an increase in the parameter φ_{0g} by 50 times.

The main equations

Energy Fundamentals of NET for Describing SPD Processes

The general model, specifically the two-level and two-mode model, taking into account the contributions of grain boundaries (GB) up to the fourth degree with respect to defect density:

$$u(h_g, h_D) = u_0 + \sum_{m=g,D}\left(\varphi_{0m}h_m - \frac{1}{2}\varphi_{1m}h_m^2 + \frac{1}{3}\varphi_{2m}h_m^3 - \frac{1}{4}\varphi_{3m}h_m^4\right) + \varphi_{gD}h_g h_D - \psi_{gD}h_g^2 h_D \quad (1)$$

where u_0, φ_{km}, φ_{gD}, ψ_{gD} are coefficients that depend on the equilibrium variables s (entropy) and ε_{ij}^e (elastic strain) as controlling parameters:

$$u_0 = \frac{1}{2}\lambda\left(\varepsilon_{ij}^e\right)^2 + \mu\left(\varepsilon_{ij}^e\right)^2, \quad (2)$$

$$\varphi_{0m} = \varphi_{0m}^* + g_m\varepsilon_{ii}^e + \left(\frac{1}{2}\bar{\lambda}\left(\varepsilon_{ij}^e\right)^2 + \bar{\mu}\left(\varepsilon_{ij}^e\right)^2\right), \quad (3)$$

$$\varphi_{1m} = \varphi_{1m}^* - 2e_m\varepsilon_{ii}^e. \quad (4)$$

Prediction of the Bilinear Stress-Strain Curve of Aluminum Alloys Using Artificial Intelligence [3-5]

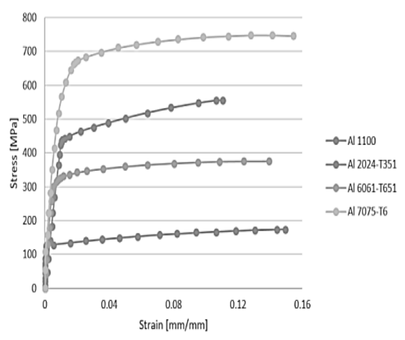
$$E = \frac{\sigma}{\varepsilon}, \quad (18)$$

$$U = U_r + T = \int_0^A \sigma \cdot d\varepsilon, \quad (19)$$

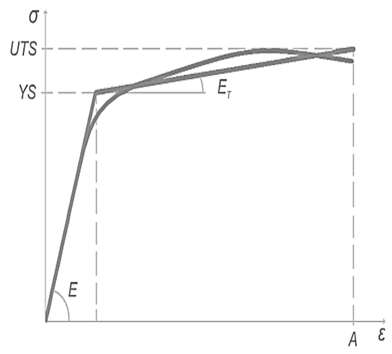
$$\varepsilon = \frac{\varepsilon}{E} + \alpha\frac{\varepsilon}{E}\left(\frac{\sigma}{\sigma YS}\right)^{n-1}, \quad (20)$$

$$\varepsilon = \frac{\sigma}{E}, \sigma \le \sigma_{YS} \quad (21)$$

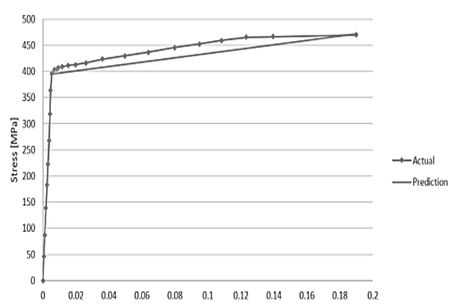
$$\varepsilon = \frac{\sigma}{E_T}, \sigma > \sigma_{YS} \quad (22)$$



Example of true stress-strain curves of some aluminum alloys.



Actual stress-strain curve and bilinear approximation for an aluminum alloy.



Actual stress-strain curve and its bilinear predicted approximation for Al 2024-T4

Artificial neural network (ANN) technology can be employed to exploit large material datasets to predict the mechanical properties of aluminum alloys. An artificial neural network can be trained to predict the bilinear approximation of the stress-strain curve of an aluminum alloy if its chemical composition and temperatures are well defined. Supervised learning methodologies require large training datasets to achieve satisfactory predictive performance. The predictive ability of a neural network improves as the dataset grows because it has more samples to learn from, and therefore, the network can approximate better the reality of the problem.

The main equations

The evolution of nonequilibrium terms of the thermodynamic potential is described by a system of differential equations:

$$\tau_{h_D}\frac{\partial h_D}{\partial t} = \varphi_{0D} - \varphi_{1D}h_D + \varphi_{gD}h_g, \quad (5)$$

$$\tau_{h_g}\frac{\partial h_g}{\partial t} = \varphi_{0g} - \varphi_{1g}h_g + \varphi_{2g}h_g^2 - \varphi_{3g}h_g^3 + \varphi_{gD}h_D. \quad (6)$$

The analytical analysis of the stationary states of the presented system (5), (6):

$$\varphi_{0D} - \varphi_{1D}h_D + \varphi_{gD}h_g = 0, \quad (7)$$

$$\varphi_{0g} - \varphi_{1g}h_g + \varphi_{2g}h_g^2 - \varphi_{3g}h_g^3 + \varphi_{gD}h_D = 0. \quad (8)$$

Similarly, we proceed for time dependencies with a nonlinear relationship:

$$\tau_{h_D}\frac{\partial h_D}{\partial t} = \varphi_{0D} - \varphi_{1D}h_D + \varphi_{gD}h_g - \psi_{gD}h_g^2, \quad (9)$$

$$\tau_{h_g}\frac{\partial h_g}{\partial t} = \varphi_{0g} - \varphi_{1g}h_g + \varphi_{2g}h_g^2 - \varphi_{3g}h_g^3 + \varphi_{gD}h_D - 2\psi_{gD}h_g h_D, \quad (10)$$

$$\varphi_{0D} - \varphi_{1D}h_D + \varphi_{gD}h_g - \psi_{gD}h_g^2 = 0, \quad (11)$$

$$\varphi_{0g} - \varphi_{1g}h_g + \varphi_{2g}h_g^2 - \varphi_{3g}h_g^3 + \varphi_{gD}h_D - 2\psi_{gD}h_g h_D = 0. \quad (12)$$

Hardening curves, including the influence of grain boundary (GB) sliding:

Taylor's relationship

$$\tau = \alpha\mu b\sqrt{h_D}, \quad (13)$$

$$\varepsilon^e = \alpha b\sqrt{h_D}. \quad (14)$$

Hall–Petch law:

$$\varepsilon^e = \varepsilon^{e0} + A\sqrt{h_g}, \quad (15)$$

Linear dependence:

$$\varepsilon^e = \varepsilon^{e1} + Bh_g, \quad (16)$$

$$\varepsilon^e = \alpha b\sqrt{h_D} - wh_g, \quad (17)$$

Conclusions

The methods of obtaining nanostructured materials, namely the methods of severe plastic deformation, have been revealed. Considering the two-defect approximation, the main relationships in terms of internal energy have been characterized, and the stages of the fragmentation process have been investigated.

The dependencies of dislocation density and grain boundaries over time have been described, as well as these dependencies with a nonlinear connection. It is shown that in this model example, dislocations have a rather sharp transition from low density values at the beginning of the SPD process to higher values corresponding to the structural-phase transition.

The dependency of external stresses on the density of grain boundaries has been described, along with this dependency with nonlinear connection. It is shown that the dependency predominantly has the form of a monotonically decreasing curve, on which there are practically no sharp changes or oscillations. At the same time, slight changes in slope are observed in the area of the structural-phase transition, which, however, may play a significant role in changing the strengthening law.

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