Modeling strengthening kinetics in metals under extreme plastic straining

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Abstract

This study utilizes the formalism of nonequilibrium evolutionary thermodynamics (NET) to describe structural evolution. The variation in internal energy is formulated through a fundamental thermodynamic identity, which balances energy flux from external sources with its dissipation through internal degrees of freedom during relaxation. We specifically model the system's response to external work and thermal driving forces. Relaxation is bifurcated into two simultaneous channels: the kinetic accumulation of lattice defects and entropy production via heat dissipation. It is established that the primary energy storage mode in the early stages is the rapid escalation of internal energy, governed by the synergetic increase in both the density and the specific energy of the defect population.

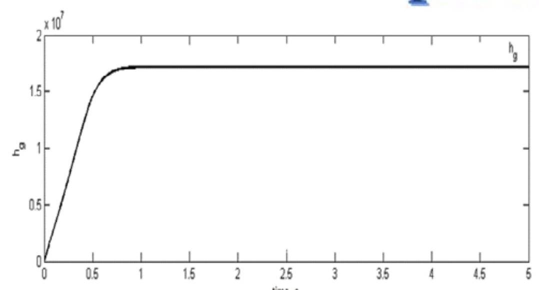
Furthermore, we evaluate the synthesis of nanostructured materials by contrasting severe plastic deformation (SPD) techniques with NET-based predictive models. Implementing a dual-defect approximation, we elucidate the constitutive relations of internal energy and the hierarchical stages of substructure fragmentation. The analysis focuses on the coupled nonlinear dynamics of dislocation ensembles and grain boundary networks. Our results indicate a sharp transition in dislocation density at the inception of SPD, characteristic of a structural phase transition. While the dislocation subsystem reaches a dynamic equilibrium (steady state) relatively early, the grain boundary density exhibits a delayed saturation, constrained by the underlying dislocation kinetics.

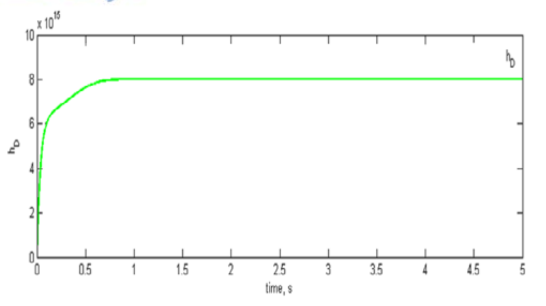
In conclusion, the work characterizes the functional dependence of yield stress on grain boundary density, accounting for nonlinear feedback loops. This relationship manifests as a monotonic decay lacking stochastic oscillations or discontinuities. However, a significant inflection point is identified within the phase transition regime, suggesting a fundamental shift in the strain hardening exponent and the overall constitutive behaviour of the material.

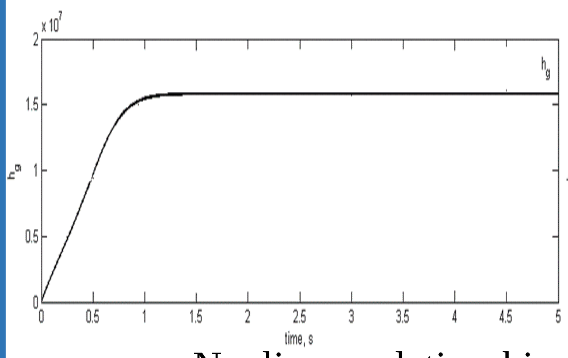
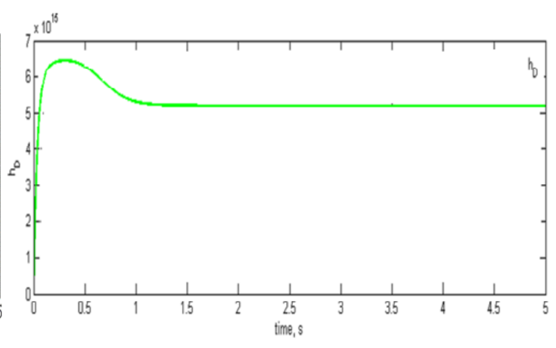
Problem statement

Within the framework of nonequilibrium evolutionary thermodynamics, we investigate the process of fragmentation of a metal structure under severe plastic deformation (SPD). Analyze the time dependencies of dislocation and grain boundaries densities 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.

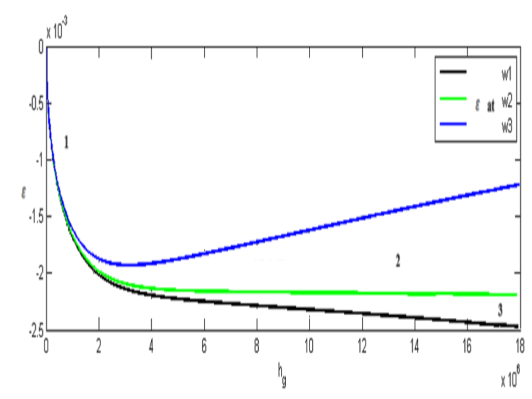
Patterns of defect formation during DIP (deformation-induced processes):

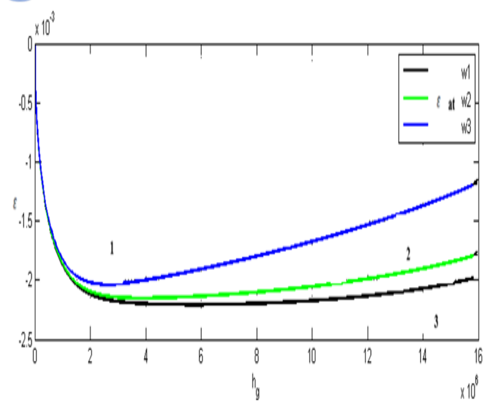

Defect kinetics $h_g(t)$.


Defect kinetics $h_D(t)$.



Nonlinear relationship

Hardening curves


Hardening curves incorporating the influence of grain boundary (GB) sliding for a linear relationship model. The transition from Hall-Petch dominance to linear/quadratic strengthening regimes is shown for various GBs intensities ($w_1 = 0$, $w_2 = 1.5 \times 10^{-11}$, $w_3 = 7 \times 10^{-11}$). In all following figures, w increases upward along the vertical axis.
1 – The Hall-Petch law
2 – Linear strengthening law
3 – Quadratic strengthening law


Hardening curves calculated using a nonlinear relationship model. The plots highlight the increased sensitivity of the deformation response to GB sliding parameters at submicroscopic scales ($w_1 = 0$, $w_2 = 1.2 \times 10^{-11}$, $w_3 = 5 \times 10^{-11}$).
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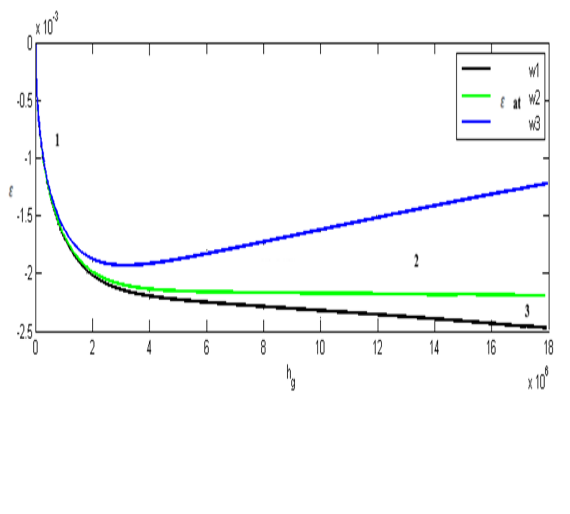

Hardening curves illustrating the competition between quadratic and linear strengthening laws under the influence of grain boundary sliding (w). The 50-fold increase in φ_{0g} highlights the accelerated structural evolution. Hardening curves, including the influence of grain boundary (GB) sliding: $w_1 = 0$, $w_2 = 1.5 \times 10^{-11}$, $w_3 = 7 \times 10^{-11}$ and with an increase in the parameter φ_{0g} by 50 times.
1 – The Hall-Petch law
2 – Linear strengthening law
3 – Quadratic strengthening law

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:

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

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

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

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

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

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

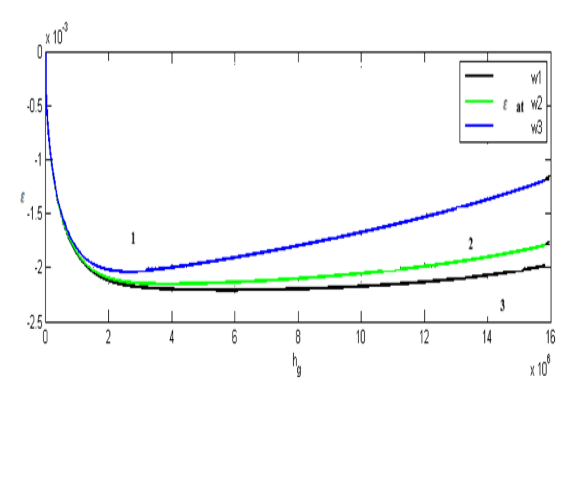
Hall–Petch law:

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

Linear dependence:

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

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


Hardening curves calculated using a nonlinear relationship model. The plots highlight the increased sensitivity of the deformation response to GB sliding parameters at submicroscopic scales ($w_1 = 0$, $w_2 = 1.2 \times 10^{-11}$, $w_3 = 5 \times 10^{-11}$).
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Conclusions

This article presents a comprehensive analysis of current approaches to the strengthening of metals, with a particular focus on nanostructured materials and severe plastic deformation (SPD) techniques. The study demonstrates that SPD methods provide effective control over structural transformations and the formation of steady-state conditions in metallic materials. The integration of phenomenological models, which combine the first and second laws of thermodynamics, enables a deeper understanding of fragmentation mechanisms and the evolution of microstructure during SPD.

The article highlights the time-dependent behaviour of dislocation density and grain boundary density, emphasizing the nonlinear relationships that govern these processes. It is shown that structural-phase transitions are characterized by abrupt changes in dislocation density, while grain boundary density continues to increase even after the stabilization of the dislocation structure. The dependence of external stress on grain boundary density is predominantly monotonic and decreasing, with minor slope variations observed in the region of the structural-phase transition, which may significantly influence the strengthening law. Practical implications are discussed, particularly regarding the importance of considering the creep threshold to ensure the reliability of aluminium alloys used in piston engine components. The proposed approach to limiting thermal loads contributes to enhanced operational reliability. The article is a theoretical model for the evolution of the defect structure in metals during severe plastic deformation (SPD) was developed based on the framework of non-equilibrium thermodynamics (NET). By integrating the first and second laws of thermodynamics, a mathematical approach was proposed to describe the fragmentation kinetics and the conditions for the formation of a steady-state structural configuration.

The key findings of the research are as follows:

1. Two-Defect Approximation: The patterns of internal energy redistribution between the dislocation subsystem and grain boundaries (GBs) were established, allowing for the identification of the fragmentation stages as a sequence of nonequilibrium structural phase transitions.
2. Stress Self-Consistency: The application of a modified Taylor relation confirmed a self-consistent feedback loop between the applied flow stress and the parameters of the steady-state structure, which determines the mechanical stability of the nanomaterial.
3. Defect Kinetics: It was revealed that the dislocation density exhibits a sharp transition (jump) at the initial stages of SPD, whereas the accumulation of grain boundary density occurs more gradually, reaching a stationary value significantly later.
4. Hardening Evolution: Analysis of the external stress dependence on the grain boundary density showed distinct slope changes within the region of the structural phase transition. This indicates a shift in the dominant hardening law as the material transitions from dislocation-mediated to grain-boundary-mediated strengthening (Hall-Petch behaviour).

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