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MECHANICS

Solid-State Stress-Induced Phase Transitions in a Material with Nanodimensional Inhomogeneities: Model and Computational Experiment

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The Landau–Ginzburg phenomenological theory is a widespread approach to the description of phase transitions [1, 2]. The main notion in this theory is the notion of the order parameter, which characterizes the atomic configuration in the material during the phase transition. In the general case, to describe the state of the medium, several order parameters can be used [3]. Based on the Landau–Ginzburg theory, some models describing phase transitions in solids were developed [4–6].

The approach to simulation of nonequilibrium solid-state stress-induced phase transitions was suggested in [7, 8]. In the context of this approach, the transformation strains of the phases, latent energy of the phase transition, dependences of elasticity moduli on order parameters, and dependence of free energy on gradients of the order parameters are taken into account. The approach is oriented to simulation of phase transitions in steels and materials with shape memory.

This approach was developed and generalized in [9, 10]. Nonlinear effects appearing under finite deformations and their redistribution were taken into account in the statement and solution of the problems [11]; not only intrinsic but also elastic deformations were considered as finite strains. The effect of nanodimensional inhomogeneities on the stressed-deformed and phase states of the body was investigated.

In this article, we further develop this approach. The problems in the dynamic statement are considered. The possibility of varying the phase state of the sample because of the formation of a new defect during the phase transition is investigated.

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1. STATEMENT OF THE PROBLEM

We consider a nonlinearly elastic body with microvoids distributed in them (circular or elliptic microholes in the case of a plane problem). It is considered that the body material can be in several phase states (for example, for the NiAl alloy, these are austenite and three martensite phases). The mechanical properties of the material in different phase states are different. During isothermal deformation, the phase transition occurs in the body, or, at least, in some part of it.

The statement of the problem is based on the theory of multiple application of large deformations.

We use n independent parameters of the order η_1, η_2, ..., η_n ($n = 2$ or $n = 3$, $0 \le \eta_k \le 1$). The free energy is specified in the form

$$\psi = A(\overset{0}{E}_e, \eta_1, \eta_2, \ldots, \eta_n) + \sum_{k=1}^{\eta} f(\eta_k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} F_{ij}(\eta_i, \eta_j),$$

where $\overset{0}{E}_e = \frac{1}{2}(\Psi_e \cdot \Psi_e^* - I)$ is the elastic deformation tensor, $\Psi_e = \Psi_t^{-1} \cdot \Psi_{0,p}$ elastic deformation gradient, $\Psi_{0,p}$ is the total deformation gradient upon going from the initial state to the pth state, and Ψ_t transformation strain gradient. Functions f and F_{ij} are specified in the form

$$f(\eta_k) = A\eta_k^2(1-\eta_k)^2 + \Delta G^{\theta}(4\eta_k^3 - 3\eta_k^4),$$

$$F_{ij}(\eta_i, \eta_j) = B\eta_i\eta_j(1-\eta_i-\eta_j)[(\eta_i-\eta_j)^2-\eta_i-\eta_j] + D\eta_i^2\eta_j^2(1-\eta_i-\eta_j) + \eta_i^2\eta_j^2(\eta_i+\eta_j)(\bar{A}-A) + \eta_i^2\eta_j^2(\eta_i T_{ij}+\eta_j T_{ji}),$$

$$\Psi_t = I + \sum_{k=1}^{n} g(\eta_k)\varepsilon_{t,k} - \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \eta_i^2\eta_j^2(\eta_i Z_{ij} + \eta_j Z_{ji});$$

here

$$Z_{ij} = (a-3)\varepsilon_{t,j} + 3\varepsilon_{t,i}, \quad \varepsilon_{t,k} = \Psi_{t,k} - I,$$

$$g(\eta_k) = a\eta_k^2(1-\eta_k)^2 + (4\eta_k^3 - 3\eta_k^4),$$

ΔG^θ, A, $\bar{A}$, a, B, and D are the specified constants (ΔG^θ is the difference between the thermal parts of the Gibbs energy of different phases).

Elastic potential A is specified in the form corresponding to the Murnaghan potential [11, 12] allowing for the dependences of elasticity moduli on the order parameters:

$$\overset{0}{A}(\overset{0}{E}_e, \eta_1, \eta_2, \ldots, \eta_n) = \frac{\lambda(\eta_1, \eta_2, \ldots, \eta_n)}{2}(E_1)^2 + \mu(\eta_1, \eta_2, \ldots, \eta_n)E_2 + C_3(\eta_1, \eta_2, \ldots, \eta_n)(E_1)^3 + C_4(\eta_1, \eta_2, \ldots, \eta_n)E_1E_2 + C_5(\eta_1, \eta_2, \ldots, \eta_n)E_3;$$

here, E_k are the invariants of tensor $\overset{0}{E}_e$;

$$\lambda(\eta_1, \eta_2, \ldots, \eta_n) = \lambda_0 + \sum_{k=1}^{n}(\lambda_k - \lambda_0)\bar{g}(\eta_k),$$

$$\mu(\eta_1, \eta_2, \ldots, \eta_n) = \mu_0 + \sum_{k=1}^{n}(\mu_k - \mu_0)\bar{g}(\eta_k),$$

$$C_m(\eta_1, \eta_2, \ldots, \eta_n) = C_m^0 + \sum_{k=1}^{n}(C_m^{(k)} - C_{m,0})\bar{g}(\eta_k),$$

$$T_{ij} = -3\left[\frac{1}{2}(\lambda_i - \lambda_0)(E_1^2) + (\mu_i - \mu_0)E_2 + (C_3^{(i)} - C_3^0)(E_1)^3 + (C_4^{(i)} - C_4^0)E_1E_2 + (C_5^{(i)} - C_5^0)E_3\right];$$

here, λ_0 and μ_0 are the Lame constants for austenite, and λ_k and μ_k at $k > 0$ are the Lame constants for martensite phases.

The equation of motion is written in the form

$$\overset{p-1}{\nabla}\cdot[(1+\Delta_{0,p-1})^{-1}\overset{p-1}{\Sigma}_{0,p}\cdot\Psi_{p-1,p}] = \rho_{p-1}\frac{\partial^2 u_p}{\partial t^2};$$

here $\overset{p-1}{\Sigma}_{0,p} = \Psi^*_{0,p-1}\cdot\overset{0}{\Sigma}_{0,p}\cdot\Psi_{0,p-1}$.

The constitutive relations correspond to the selected potential:

$$\overset{0}{\Sigma}_{0,p} = \frac{\partial \overset{0}{A}(\overset{0}{E}_e, \eta_1, \eta_2, \ldots, \eta_n)}{\partial \overset{0}{E}_e}.$$

The kinematic relations have the form [11]

$$\overset{0}{E}_e = \frac{1}{2}(\Psi_e\cdot\Psi_e^* - I), \quad \Psi_e = \Psi_t^{-1}\cdot\Psi_{0,p},$$

$$\Psi_{0,p} = \Psi_{0,p-1}\cdot\Psi_{p-1,p}, \quad \Psi_{p-1,p} = I + \overset{p-1}{\nabla}u_p;$$

here, u_p is the vector of displacements from the $(p-1)$th state into the pth state.

Evolution equations for order parameters have the form

$$\frac{\partial\eta_k}{\partial t} = 2\Lambda\beta\overset{p-1}{\nabla}\cdot(\overset{p-1}{\nabla}\eta_k) + \Lambda X_k, \quad k = 1, 2, \ldots, n;$$

here, $X_k = P\cdot\Psi_e^* : \frac{\partial\Psi_t^*}{\partial\eta_k} - \frac{\partial\Psi}{\partial\eta_k}\Big|_{\overset{0}{E}_e}$, $k = 1, 2, \ldots, n$ are the moving forces of the phase transition, $P = \overset{0}{\Sigma}_{0,p}\cdot\Psi_{0,p}$ is the first tensor of the Piola stresses, Λ is the kinetic coefficient characterizing the rate of the phase transition, and β is the constant characterizing the width of the spread phase interface. The value of this constant was determined in [8] by comparison of an exact solution of the static Landau–Ginzburg equation with the experimental data on the width of the transition layer at the interface between the martensite phases for the $Ni_{65}Al_{35}$ alloy [13], which is in the range from one to several interatomic distances.

At the outer boundary of the body, stresses $\sigma_{0,p} = \sigma_\infty$ are specified, and contours of the holes are considered to be free of loads: $\overset{p-1}{N}\cdot\overset{p-1}{\Sigma}_{0,p} = 0$; here, $\overset{p-1}{N}$ is the vector of the unit normal. For the order parameters on the outer boundary and hole contours, conditions are specified $\overset{p-1}{N}\cdot(\overset{p-1}{\nabla}\eta_k) = 0$, $k = 1, 2, \ldots, n$.

The suggested set of equations allows us to determine the phase state of the medium during deformation.

The formulated problem is a coupled problem of nonlinear elasticity and the theory of phase transitions [14]. When solving it, the mutual influence of the stressed-deformed and phase states of the medium in the course of the evolution of the latter should be taken into account.

2. MODEL CALCULATIONS

To solve the problem under consideration, we cannot use the commercial finite-element packages since

this problem is coupled, and deformations are finite and redistribute during the phase transition. Therefore, for numerical calculations, we developed specialized software based on the finite element method [11, 15]. We used linear triangle elements.

The material with two order parameters was used for the calculations. The main phases were austenite (A) and two martensite phases: M_1 and M_2. Values $\eta_1 = \eta_2 = 0$ correspond to austenite, $\eta_1 = 1$ and $\eta_2 = 0$ correspond to the first martensite phase, and $\eta_1 = 0$ and $\eta_2 = 1$ correspond to the second martensite phase. We used the constant for the material calculated in [7] for the NiAl alloy based on the results of simulation by the methods of molecular dynamics. The density of austenite in the deformed state $\rho_0 = 6000$ kg/cm^3. The elasticity moduli of austenite are $\lambda_0 = 144$ and $\mu_0 = 74$ (henceforth, the values of all elasticity moduli and loads are given in gigapascals, and all values of dimensionality of the length are given in nanometers). The elasticity moduli for both martensite phases are identical: $\lambda_1 = \lambda_2 = 379$, $\mu_1 = \mu_2 = 134$. These moduli were calculated by averaging over directions of the moduli presented in [7]. The martensite phases differ from each other only by the direction of transformation strains. The transformation strains of the first martensite phase are $\Psi_{11} = 1.215$, $\Psi_{22} = \Psi_{33} = 0.922$. Transformation strains of the second martensite phase are $\Psi_{11} = \Psi_{33} = 0.922$, $\Psi_{22} = 1.215$. Other parameters are $\beta = 2.59 \times 10^{-10}$ N, $\Delta G^0 = -0.315$ GPa, $A = 0.8$ GPa, $\bar{A} = 5.32$ GPa, $\beta = 0$, and $D = 0.5$ GPa. Calculations were performed for the case of plane deformation.

We further present certain results of solution of model problems. In all these problems, we considered a quadrate sample with side l, the center of which coincided with the origin of the coordinates.

Problem 1. Sample size $l = 26.6$; one circular hole with radius $r = 5$ was arranged in the center of the sample. Around the hole, the inclusion in a form of a circular ring with outer radius $R = 6.67$ was arranged. The inclusion was a mixed nucleus of phases M_1 and M_2 ($\eta_1 = 0.1$, $\eta_2 = 0.1$). In the rest of the sample, at the initial point in time, $\eta_1 = \eta_2 = 0$. The load had uniform tension ($p_x = p_y = 15$); in this problem, the load was applied to the body with the hole already present. The problem was solved in a dynamic statement with step in time $\tau = 1.5 \times 10^{-5}$ ns. The distribution of order parameter η_1 at the point in time $t = 0.003045$ ns is shown in Fig. 1. The distribution of η_2 is obtained from that presented in Fig. 1 by rotation for 90° with respect to the sample center.

As is evident from Fig. 1, the regions of the first phase of martensite were formed from the top and from the bottom with respect to the hole (in the direction of the axis y from its center). In the direction of the axis x from the hole center (to the left and to the right from the center in Fig. 1), the regions of the second phase of martensite formed. The distribution of the order parameter in each of the formed regions is nonuniform. Near the hole, the zone is in each such region where the order parameter is close to unity, while in the other part of each region, the order parameter is close to 0.5.

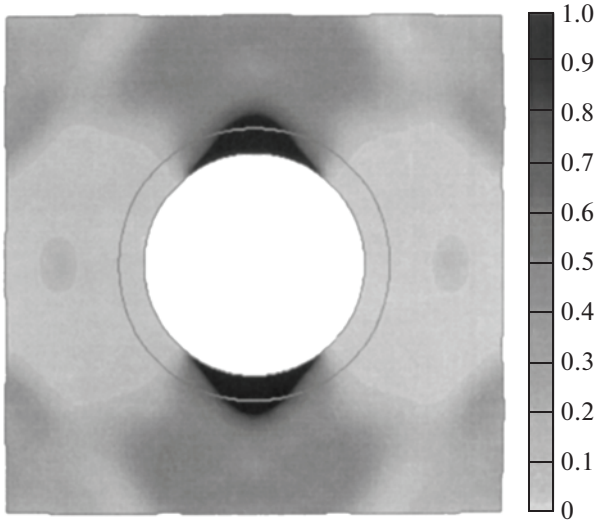

Fig. 1. Distribution of η_1 in the sample for problem 1 at the point in time $t = 0.003045$ ns.

Problem 2. Sample size $l = 40$. Each order parameter at the initial point in time in each finite element was specified as a random quantity distributed uniformly in the range from 0 to 0.1; the element area was no larger than 0.13 nm^2. The load is the uniaxial tension ($p_x = 10$, $p_y = 0$). T the point in time $t_1 = 44 \times 10^{-5}$ ns after applying the load, a hole with radius $r = 5.5$ formed in the sample center. The problem was solved in the quasi-static statement with the step in time $\tau = 4 \times 10^{-5}$ ns. In a certain time after the formation of the hole, the stressed-deformed and phase state of the sample close to the steady state was attained. In this state, $\eta_2 = 0$ was established over the whole sample, while the distribution of η_1 after the establishment was nonuniform.

Calculations were also performed for the case when the hole is not formed in the sample. In both cases, nonuniformities of the phase state in the form of strips elongated in the tension direction were formed in the sample. The results of calculations showed that the formation of the hole substantially affects the phase state near it. The distribution of η_1 in the steady state for the case when the hole is formed in the sample is shown in Fig. 2. This distribution is asymmetric. This

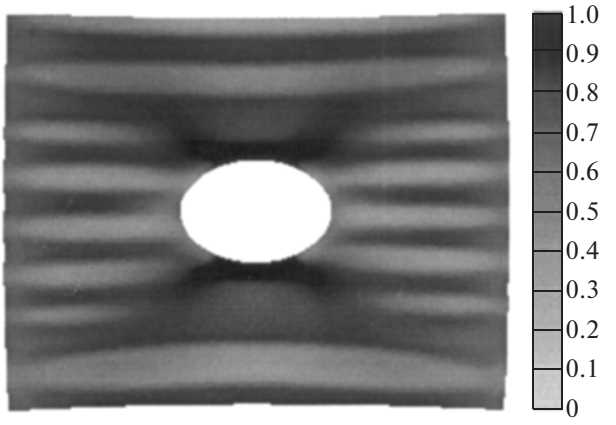

Fig. 2. Steady-state distribution of η_1 in the sample for problem 2.

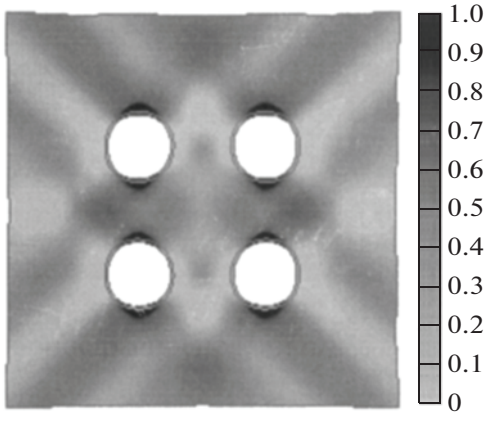

Fig. 3. Steady-state distribution of η_1 in the sample for problem 3.

can apparently be explained by the fact that the hole formed at the point in time when there was a nonuniform distribution of the phase state in the form of asymmetric strips because of the random character of the initial distribution of the order parameters already formed in the sample.

Problem 3. Sample size $l = 56$; four symmetrically arranged holes of identical radii $r = 4$ formed in the sample after loading. The coordinates of the centers of holes are $x_c = \pm 9$, $y_c = \pm 9$. An inclusion shaped like a circular ring with outer radius $R = 4.5$ was arranged around each hole. The inclusion was a mixed nucleus of the phases M_1 and M_2 ($\eta_1 = 0.1$, $\eta_2 = 0.1$). In the last part of the sample, at the initial point in time, $\eta_1 = \eta_2 = 0$. The load is the uniform tension ($p_x = p_y = 15$). The problem was solved in a quasi-static statement. In a certain time after the formation of holes, a stressed-deformed and phase state of the sample close to the steady-state was attained. The distribution of η_1 in the steady state is shown in Fig. 3. The distribution of η_2 is obtained from that presented in Fig. 3 with rotation by 90° with respect to the sample center.

Let us note that for all problems considered above, no complete transition into one of the martensite phases occurred in most of the samples, i.e., the corresponding order parameter did not reach unity. This is apparently associated with the fact that for the plane-deformed state, limitation of the deformation is imposed, and the potential has minima points in this case; these points differ from its minima points in the absence of these limitations.

Thus, in this work, the kinetic model of the phase transition at finite deformations based on the Landau–Ginzburg theory is realized. The model takes into account the latent energy of the phase transition, the dependence of elastic properties of the material on the order parameters, and the finite intrinsic and elastic deformations.

The results of calculations show the possibility of formation of steady-state nanostructures (regions with a nonuniform distribution of order parameters) in the body of steady-state nanostructures.

It is established that the formation of the defect during the phase transition leads to a substantial variation in the phase state in the vicinity of this defect.

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REFERENCES

1. L. D. Landau and E. M. Lifshits, *Theoretical Physics* (Fizmatlit, Moscow, 2002), Vol. 1 [in Russian].
2. L. D. Landau and I. M. Khalatnikov, Dokl. Akad. Nauk SSSR **96** (3), 469 (1954).
3. Yu. A. Izyumov and V. N. Syromyatnikov, *Phase Transitions and Symmetry of Crystals* (Nauka, Moscow, 1984) [in Russian].
4. P. Toledano and V. Dmitriev, Reconstructive Phase Transitions. New Jersey: World Sci. (1996).
5. Y. Wang and A. G. Khachaturyan, Acta Metal. Mater. **45**, 759 (1997).
6. V. I. Kondaurov, Dokl. Akad. Nauk **396** (2), 194 (2004).
7. V. I. Levitas and D. L. Preston, Phys. Rev. B: **66**, 134207 (2002).
8. V. I. Levitas, D. L. Preston, and D.-W. Lee, Phys. Rev. B: **68**, 134201 (2003).
9. V. I. Levitas, V. A. Levin, K. M. Zingerman, and E. I. Freiman, Phys. Rev. Lett. **103**, 025702 (2009); republished in Virtual J. Nanoscale Sci. Technol. **20** (3), 2009.

10. V. A. Levin, V. I. Levitas, V. V. Lokhin, and K. M. Zingerman, in *Modern Problems of Mathematics and Mechanics* (Mosk. Gos. Univ., Moscow, 2009), Vol. 2, pp. 49–57 [in Russian].
11. V. A. Levin, V. V. Kalinin, K. M. Zingerman, and A. V. Vershinin, *Development of Defects during Finite Deformations. Computer and Physical Simulation* (Fizmatlit, Moscow, 2007) [in Russian].
12. A. I. Lur'e, *Nonlinear Elasticity Theory* (Nauka, Moscow, 1980) [in Russian].
13. Ph. Boullay, D. Schryvers, and J. M. Ball, Acta Mater. **51**, 1421 (2003).
14. V. I. Kondaurov and V. E. Fortov, *Foundations of Thermal Mechanics of the Condensed Medium* (MFTI, Moscow, 2000) [in Russian].
15. O. C. Zienkiewicz and R. L. Taylor, *The Finite Element Method. Vol. 2. Solid Mechanics* (Butterworth-Heinemann, Oxford, 2000).

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