

**DERIVATION OF A UNIVERSAL RELATION  
BETWEEN TANGENTIAL STRESS  
AND SHEAR STRAIN INTENSITIES  
IN DESCRIBING REVERSIBLE MARTENSITIC DEFORMATION  
WITHIN THE FRAMEWORK OF A SYNTHETIC MODEL**

I. M. Goliboroda and K. N. Rusinko

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In designing and applying new structural materials, one often encounters the problem of predicting and taking into account nonlinear strains caused by reversible martensitic transformations. These transformations proceed by cooperative motion of atoms and give rise to a wide range of peculiar phenomena (superelasticity, shape memory effect, transformation elasticity, etc.), which alter radically the material properties and lead to new opportunities for their practical use. Thus, it is obvious that we need a mathematical model that allows wide practical application and enables one to describe and predict the deformation behavior of polycrystals with allowance for the aforementioned phenomena.

The plastic deformation model based on the synthesis of slip concepts and flow theory is rigorous, simple, and mathematically justified [1, 2]. Therefore, it makes sense to develop it further to describe and predict the deformation behavior of modern structural materials under complex temperature-force regimes of loading with allowance for the essential microstructural properties of the phenomena in question. The synthetic model is used below to describe the nonlinear reversible deformation caused by martensitic reactions of the first kind.

**Defining Relations of the Model.** To consider the essential properties of the phenomena at the microscopical level, recall some well-known principles [3]. The laws of reversible phase transitions are described by a diagram (Fig. 1) which is plotted in the coordinate system of the relative amount of low-temperature (martensite) phase  $\Phi$  and effective temperature  $T^*$ . In a given microvolume,  $\Phi = 0$  and  $\Phi = \Phi_0$  correspond to the initial and final moments of the direct reaction of transition from the high-temperature phase to the low-temperature one (from now on, these phases will be called austenite and martensite, respectively). The points  $M_{ini}$  and  $M_f$ ,  $A_{ini}$  and  $A_f$  correspond to the characteristic initial and final temperatures of the direct and reverse reactions. The reason for introducing the concept of effective temperature (the equation for it will be given below) and for plotting the diagram in the above coordinate system is that the characteristic temperatures of the reactions are shifted under the applied loading. The effective temperature reflects the Clausius-Clapeyron principle [3, 4] of the influence of strength loading on the kinetics of martensitic transitions and ensures nondependence of the characteristic temperatures, as material parameters, on the applied loading.

To describe the reaction kinetics in accordance with Fig. 1 we use the equality [3]

$$\begin{aligned} \dot{\Phi} = & -\dot{T}^* \{ H(\Phi_0 - \Phi) H(-\dot{T}^*) H[M_{ini} - \Phi(M_{ini} - M_f) - T^*] (M_{ini} - M_f)^{-1} \\ & + H(\Phi) H(\dot{T}^*) H[T^* - A_f + \Phi(A_f - A_{ini})] (A_f - A_{ini})^{-1} \} \end{aligned} \quad (1)$$

( $H$  is a Heaviside function). It was assumed that the kinetics of development of the phase reaction is essentially independent of the type of stress state [5].

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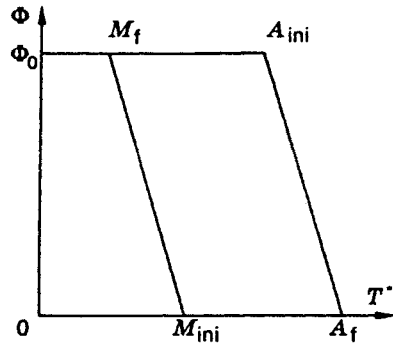


Fig. 1

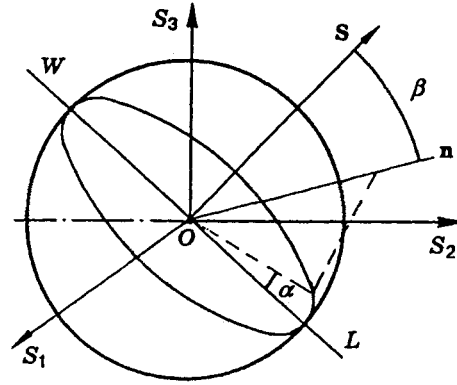


Fig. 2

Martensitic transformation of the lattice is usually accompanied by deformation of a shear nature (in most cases, dilatation effects are either absent or can be ignored [5–8]). Since the phase microstrain tensor arising in the microvolume considered is determined by the transformation (distortion) of the crystal lattice, the following relationship holds for the phase microstrain parameter [3]:

$$\varphi = D_{13}\Phi, \quad (2)$$

where  $D_{13}$  is the shear tensor component of the crystal lattice distortion due to the phase transition.

Because of the shear nature of the martensitic reaction, it makes sense to use the model based on the concept of slipping to describe the class of phenomena in question. In the concept of slipping [9], irreversible deformation is due to shears in the chosen slipping systems. Likewise, in the phenomenological interpretation used here, the strain magnitude depends upon translation of planes in the five-dimensional space of Il'yushin deviators [10]. Each of the planes is put in correspondence with a definite slipping system (a normal to the plane and a direction in the plane). The planes are displaced under the action of the stress vector  $\mathbf{S}$ , whose components are determined by the stress deviator components (here and below, we use the principles and notation of [2])

$$S_1 = \frac{3}{2}(S_{zz} + S_{xx}), \quad S_2 = \frac{\sqrt{3}}{2}(S_{zz} - S_{xx}), \quad S_3 = \sqrt{3}S_{xz}, \quad S_4 = \sqrt{3}S_{yz}, \quad S_5 = \sqrt{3}S_{xy}. \quad (3)$$

If loading is performed in a three-dimensional subspace of the aforementioned deviator space, determined by the vector components  $S_1$ ,  $S_2$ , and  $S_3$  (Fig. 2), the strain is found uniquely from the displacement of traces of these planes in the three-dimensional subspace. We denote a normal to a plane in the five-dimensional space by  $\mathbf{N}$ , a normal to its trace in the three-dimensional subspace by  $\mathbf{n}$ , and the angle between the normals  $\mathbf{N}$  and  $\mathbf{n}$  by  $\lambda$

$$N_k = n_k \cos \lambda, \quad k = 1, 2, 3. \quad (4)$$

The orientation of the vector  $\mathbf{S}$  under proportional loading in the space of the components  $S_1$ ,  $S_2$ , and  $S_3$  is determined by the direction cosines  $n_k^0$ . The orientation of the normal  $\mathbf{n}$  is defined in a spherical coordinate system that is connected with the loading vector  $\mathbf{S}$  by means of the angles  $\beta$  and  $\alpha$  ( $\beta$  is the angle between  $\mathbf{S}$  and  $\mathbf{n}$ , and  $\alpha$  is the angle between the projection of  $\mathbf{n}$  onto the plane  $W$  perpendicular to  $\mathbf{S}$  and the line  $L$  of intersection of the plane  $W$  with the coordinate plane  $S_1OS_2$ ). In fact, this choice of coordinate angles leads to coincidence of the coordinate axes with the loading vector  $\mathbf{S}$  and to a simpler expression for the direction cosines  $n_k$  of the normal  $\mathbf{n}$  in terms of the direction cosines of the loading vector  $n_k^0$  (due to invariance with respect to the angle  $\alpha$ ) [2].

In the basic synthetic theory of plasticity, the action of the loading vector causes the planes in the deviator space move as a rigid unit (each plane can be put in correspondence with a point in the space of

the variables  $\alpha$ ,  $\beta$ , and  $\lambda$ ) and thus governs the transformation of the loading surface. This surface and the boundaries of its transformed region can be found from the plasticity condition [2]. In the present model, the temperature level and the loading vector determine the region in which martensitic transition in the space of the angular coordinates  $\alpha$ ,  $\beta$ , and  $\lambda$  is realized. The exact boundaries of the region can be found from (1).

When applied at the macrolevel to averaged deformations, the coordinate system in question makes it possible to write an expression for the strain vector components (which is constructed in the five-dimensional space of deviators in the same manner as the loading vector) at the macrolevel in the form

$$\varepsilon_k^{\text{ph}} = \int_0^t \iiint_{\Omega} N_k \dot{\varphi} f(\Omega) ds d\Omega, \quad (5)$$

where  $\Omega(\alpha, \beta, \lambda)$  is the region in which the phase reaction occurs ( $0 \leq \alpha \leq 2\pi$ ,  $0 \leq \beta \leq \pi$ , and  $0 \leq \lambda \leq \pi/2$ );  $f(\Omega)$  is a macroanisotropic parameter. For a macroanisotropic medium,  $f(\Omega) = 1/(2\pi^2)$ .

Taking into account (4) and the definition of the coordinate angles, we find

$$\varepsilon_k^{\text{ph}} = \frac{n_k^0}{2\pi^2} \int_0^t \iiint_{\alpha \beta \lambda} \dot{\varphi} \cos^2 \beta \cos \lambda \sin \beta d\alpha d\beta d\lambda dS. \quad (6)$$

According to the assumptions made, the above effective reaction temperature can be written in a form similar to [3]

$$\dot{T}^* = \dot{T} - \frac{T_0}{q_0} D_{13} (\dot{\mathbf{S}}, \mathbf{N}). \quad (7)$$

Here,  $q_0$  is the thermal effect of reaction;  $T_0$  is the temperature of thermodynamic equilibrium of the phases; the second term on the right-hand side corresponds, as in [3], to the work of microstresses on shear strain in the lattice.

Using (4), the properties of the scalar product of the vectors  $\dot{\mathbf{S}}$  and  $\mathbf{N}$ , and the definition of the angles  $\beta$  and  $\lambda$ , relation (7) can be rewritten as

$$\dot{T}^* = \dot{T} - \frac{T_0}{q_0} D_{13} |\dot{\mathbf{S}}| \cos \beta \cos \lambda. \quad (8)$$

Relations (1), (2), (6), and (8) make it possible to describe nonlinear deformation caused by reversible martensitic reactions of the first kind under proportional loading.

**Realization of the Model for the Case of Isothermal Martensite Reaction.** The material is assumed to be entirely in the austenite state at  $T = \text{const} > M_{\text{ini}}$ , with an increasing external loading applied to it. A region  $A$ , in which the right-hand side of (8) is negative, appears in the space specified by the angles  $\alpha$ ,  $\beta$ , and  $\lambda$ . In this region,  $T^*$  decreases ("cooling" occurs). Under certain loading, the equality  $T^* = M_{\text{ini}}$  holds and a direct reaction will start. In the remaining part of the space, i.e., region  $B$ , the inequality  $T^* > 0$  holds, i.e., "heating" occurs. The region  $A$ , in which the effective temperature decreases, is bounded by the angles  $0 \leq \alpha \leq 2\pi$ ,  $0 \leq \beta \leq \pi/2$ , and  $0 \leq \lambda \leq \pi/2$ , and is an upper hemisphere (Fig. 3). In this region, the relation

$$\dot{\Phi} = K \dot{S} \cos \beta \cos \lambda H(\Phi_0 - \Phi) H(M_{\text{ini}} - T + KS \cos \beta \cos \lambda - \Phi(M_{\text{ini}} - M_{\text{f}}))(M_{\text{ini}} - M_{\text{f}})^{-1}, \quad (9)$$

holds, where  $S = |\mathbf{S}|$  is the length of the vector  $\mathbf{S}$ ;  $K = T_0 D_{13} / q_0$ .

From relation (9), equating the argument of the third Heaviside function to zero and taking into account that  $\Phi = 0$  prior to the beginning of the martensitic transition, we determine the stress  $S_{\text{ini}}$  at which the phase reaction starts (at the point  $\beta = 0$  and  $\lambda = 0$ ):

$$S_{\text{ini}} = \frac{T - M_{\text{ini}}}{K},$$

and find boundary angles that determine the region in which the reaction is realized as the stress increases (Fig. 3a):

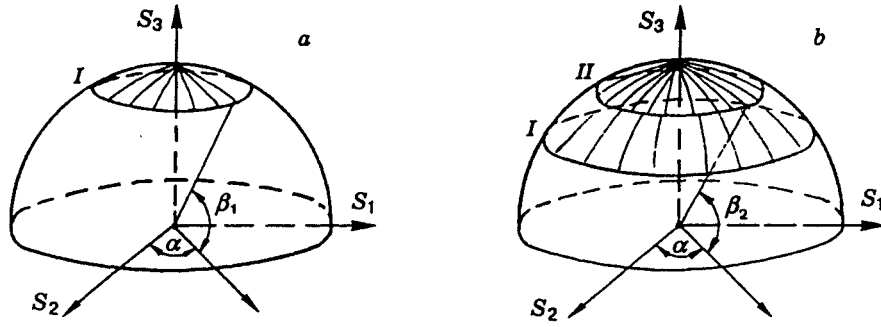


Fig. 3

$$\cos \beta_1 = \frac{T - M_{ini}}{KS} = \frac{S_{ini}}{S}, \quad \cos \lambda_1 = \frac{\cos \beta_1}{\cos \beta}. \quad (10)$$

According to (8) and (10), formula (6) takes the form

$$\varepsilon_k^{ph} = \frac{KD_{13}n_k^0}{2\pi^2 a} \int_0^t ds \int_0^{2\pi} d\alpha \int_0^{\beta_1(S)} \cos^2 \beta \sin \beta d\beta \int_0^{\lambda_1(\beta)} \cos^2 \lambda d\lambda$$

at  $a = M_{ini} - M_f$ .

It is usually assumed that  $\Phi_0 = 1$ . We set  $\Phi_0 = 2$ , because in the case of high-temperature (austenite) superelasticity, martensite crystals which have appeared in the subregion in which the reaction proceeds can grow into the subregion  $B$ , in which this reaction is prohibited [3]. In accordance with relation (9) and the requirement of  $\Phi_0 = 2$ , we define the stress  $S_0$  at which the reaction in the point region ( $\beta = 0$  and  $\lambda = 0$ ) terminates;  $S_0 = (T - 2M_{ini} + M_f)/K$ . The boundary angles characterizing the internal boundary of the region in which the reaction proceeds with a further increase in stress (Fig. 3b) is written as

$$\cos \beta_2 = \frac{T - 2M_{ini} + M_f}{KS} = \frac{S_0}{S}, \quad \cos \lambda_2 = \frac{\cos \beta_2}{\cos \beta}.$$

It the averaging, integration is performed over the indicated region of realization of the reaction. Thus, two regions appear on the hemisphere: region I, defined by the angles  $\beta_1$  and  $\beta_2$ , in which the inequalities  $0 < \Phi < 2$  hold, and region II, defined by the angle  $\beta_2$ , in which  $\Phi = 2$  and the direct reaction has completed.

For  $S > S_0$ , the increment of the phase deformation is given by the formula

$$\varepsilon_k^{ph} = \frac{KD_{13}n_k^0}{6\pi a} \left[ S \left[ \arccos \left( \frac{S_{ini}}{S} \right) - \arccos \left( \frac{S_0}{S} \right) \right] + 2 \left( \frac{S_0}{S} \sqrt{S^2 - S_0^2} - \frac{S_{ini}}{S} \sqrt{S^2 - S_{ini}^2} \right) + \left( S_{ini}^2 \ln \left| \frac{S + \sqrt{S^2 - S_{ini}^2}}{S_{ini}} \right| - S_0^2 \ln \left| \frac{S + \sqrt{S^2 - S_0^2}}{S_0} \right| \right) \frac{1}{S^3} \right].$$

The strain vector and strain deviator components are related by formulas similar to (3). The total phase strain (for pure shear and uniaxial tension, respectively) is  $\varepsilon_{zz} = D_{13}/(\pi\sqrt{3})$ ,  $\varepsilon_{xx} = 2D_{13}/(3\pi)$ .

If we begin to decrease the applied loading after the magnitude  $S = S_m$  is reached, "heating" will occur in the same region of the coordinate space  $A$ , according to (5). When the effective temperature corresponding to the onset of the reverse reaction is reached, reverse transformation of loaded martensite into austenite occurs, which is accompanied by the vanishing of strain.

The reverse reaction starts along the line  $\beta = \beta_2$  [at  $S = S_m (T - A_{ini} + 2(A_f - A_{ini})) / (KS_0)$ ], and then its region of realization extends up over the region in which the direct reaction has already ceased and  $\Phi = 2$  and down over the region in which  $0 < \Phi < 2$ . The reverse reaction will cover the entire region II (will

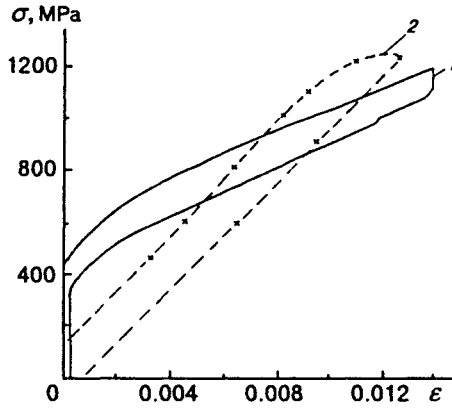


Fig. 4

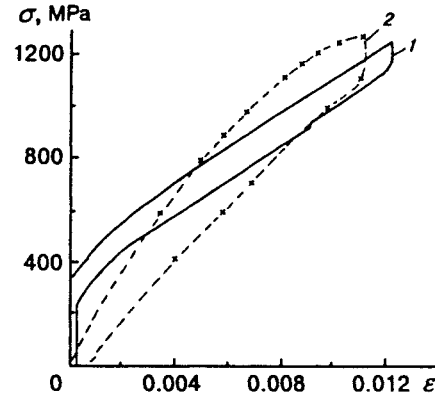


Fig. 5

reach its upper point  $\beta = 0$ ) for  $S = (T - A_{\text{ini}} + 2(A_f - A_{\text{ini}}))/K$  and reach the lower boundary of region I specified by the line  $\beta = \beta_1$  for  $S = S_m(T - A_f)/(K S_{\text{ini}})$ . Termination of the reverse transformation (because of its complete transition to austenite) begins from the line  $\beta = \beta_1$  and ceases completely for  $S = (T - A_f)/K$ . Expressions for the boundary angles and strain after loading have a form similar to the corresponding formulas during loading.

#### Reduction of Constitutive Relations of the Model to the Relations of Deformation Theory.

Formula (6) can be written as

$$\varepsilon_k^{\text{ph}} = n_k^0 F(S). \quad (11)$$

Bearing in mind that the relation  $\sqrt{\varepsilon_k^{\text{ph}} \varepsilon_k^{\text{ph}}} = (\sqrt{3}/2)\gamma^{\text{ph}}$  (where  $\gamma^{\text{ph}}$  is the intensity of shear strain caused by the phase reactions) holds for the phase strain component, we obtain  $\gamma^{\text{ph}} = (2\sqrt{2}/3)F(S)$ .

Taking into account that  $S = (3/\sqrt{2})\tau$  ( $\tau$  is the tangential stress intensity), we recast formula (11) as  $\varepsilon_k^{\text{ph}} = \gamma^{\text{ph}} S n_k^0 / (2\tau)$ .

Adding elastic strain components and moving from the vector components to the deviator components, we write  $e_{ij} = S_{ij}/(2G'(\tau))$ ,  $G'(\tau) = \gamma^{\text{ph}}/\tau + 1/G$  ( $G$  is the elastic shear modulus).

Thus, under the above assumptions, the constitutive relations of the model become analogous to the relations in the deformation theory of plasticity [11].

The universal relation between  $\tau$  and  $\gamma^{\text{ph}}$  is written as

$$\gamma = \frac{\tau}{G} + \frac{\sqrt{2}KD_{13}}{9\pi(M_{\text{ini}} - M_f)} \left\{ S \left[ \arccos\left(\frac{S_{\text{ini}}}{S}\right) - \arccos\left(\frac{S_0}{S}\right) \right] + \left[ S_{\text{ini}}^3 \ln \left| \frac{S + \sqrt{S^2 - S_{\text{ini}}^2}}{S} \right| - S_0^3 \ln \left| \frac{S + \sqrt{S^2 - S_0^2}}{S_0} \right| \right] / S^3 + 2 \left[ S_0 \sqrt{S^2 - S_0^2} - S_{\text{ini}} \sqrt{S^2 - S_{\text{ini}}^2} \right] \right\},$$

where  $\gamma$  is the shear strain intensity.

**Comparison with Experiment.** Calculations were conducted for iron-nickel alloys with the reversible  $\alpha \rightleftharpoons \gamma$  transformation. Figures 4-7 show results of the calculations of the  $\sigma - \varepsilon$  diagrams under uniaxial tension (deflection of a plastic sample loaded by the three-point bending scheme) and under unloading for Ni295Co18Ti6Fe alloy at various holding temperatures:  $T = 293, 273, 263,$  and  $243$  K (Figs. 4-7, respectively). In accordance with the data of [12], the characteristic temperatures were as follows  $M_{\text{ini}} = 225$  K,  $M_f = 150$  K,  $A_{\text{ini}} = 162$  K, and  $A_f = 237$  K. In the calculations, we used  $T_0 = 160$  and  $K = 0.173$ .

As follows from the figures, there is good qualitative and quantitative agreement between the calculated results (curves 1) and experimental results (curves 2 [12]).

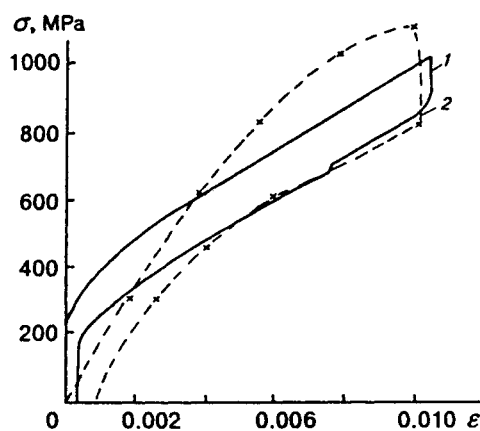


Fig. 6

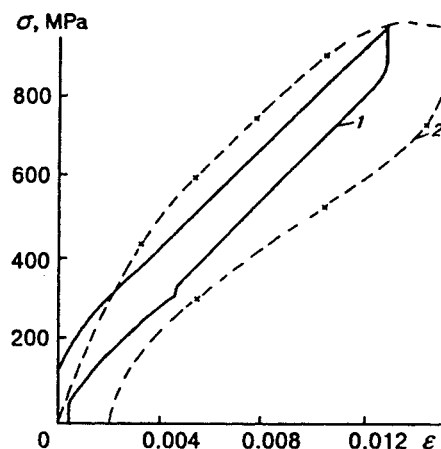


Fig. 7

**Conclusion.** The concept of slipping can be used in designing modern phenomenological models for the nonlinear deformation of polycrystals of various nature.

Among the approaches based on the concept of slipping, the synthetic approach is one of the most effective and mathematically justified.

The proposed synthetic model of phase deformation was used to describe a reversible isothermal martensitic reaction. The process of accumulation and recovery of strain under loading and unloading was described. Allowance for the microstructural peculiarities of martensitic transformations leads to understanding of macroscopic regularities in the deformation behavior of polycrystals. Use of the above averaging method enables one to describe analytically reversible changes in material properties for various types of stressed states. A universal relationship between the tangential stress and shear strain intensities is derived. The constitutive relations of the model are brought to a form analogous to the relations of the deformation theory of plasticity. Good qualitative agreement with the experimental data was obtained.

In addition to the transition considered, phase reactions of the first kind under different strength and thermal conditions can be described within the framework of this model.

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