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SIMULATION

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SYMMETRIC MODEL EVALUATION OF THE RESOURCE OF ELASTIC ENERGY STORED BY AN ENSEMBLE OF SELF-SIMILAR MARTENSITE CRYSTALS

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Resource of stored elastic energy is evaluated with the help of a symmetric model of orthogonal joining of crystals, which makes it possible to compute the number of generations of martensite crystals and the fraction of the formed martensite (the integral one and for any of the generations). It is shown that the resource of the stored elastic energy for twinned crystals may grow by an order of magnitude as compared to the variant when twins are absent; the increase with respect to the starting values of the resource amounts to almost ten orders of magnitude.

Key words: critical grain size, number of generations of crystals, volume fraction of martensite, resource of stored energy.

INTRODUCTION

In any alloy undergoing a martensitic transformation (MT) with features of phase transformation of the first kind the shape of the region of rearrangement of the lattice changes and the volume changes accordingly. Inevitably, this gives rise to elastic energy localized both in the volume of the appearing phase (martensite) and in the untransformed volume of the initial phase (austenite). Typically enough, the martensite crystals nucleated the fist have the largest size and penetrate the volume of the initial grain (or single crystal). As a result, the subsequent crystals have to form in austenitic volumes with smaller sizes. The MT process develops below the point of phase equilibrium T_0 in the temperature range $M_s - M_f$ (M_s and M_f are the temperatures of the start and finish of the MT, respectively). The transformation stops when fragments of retained austenite attain some minimum size L_{min} (of the same order as the critical grain size D_{cr}). Depending on the specific variant of the transformation and on the composition of the alloy the values of $M_s - M_f$, just like L_{min}, can vary considerably. For example, in iron-base alloys with concentration C of the second component not belonging to the neighborhood of special concentration C^* (at $C \to C^*$, $M_s \to 0$ K, $L_{min} \to \infty$) for martensitic $\gamma \to \alpha$ transformations the typical values are $L_{min} \sim (0.1 - 1)$ μm, whereas for the alloys based on titanium nickelide $L_{min} \sim 20$ nm. The arising hierarchy of crystals of different generations possesses features of statistical likelihood. In the dynamic theory of heterogeneous nucleation and wave growth of crystals [1, 2] a relation

$$d \sim 10^{-2} L_{fr}. \qquad (1)$$

holds for the transverse size d of the initial excited state in the form of an elongated fluctuating parallelepiped (that specifies the thickness of thin-plate crystals) with size L_b of the volume free of fault.

Using Eq. (1) and taking into account the possibility of size broadening of the crystals we have suggested in [2, 3] a simple symmetric model of cross-like joining of crystals, which reflects correctly the variation of the scale of the free volume in the transformation and is convenient for estimating the fractions of transformed and retained austenite.

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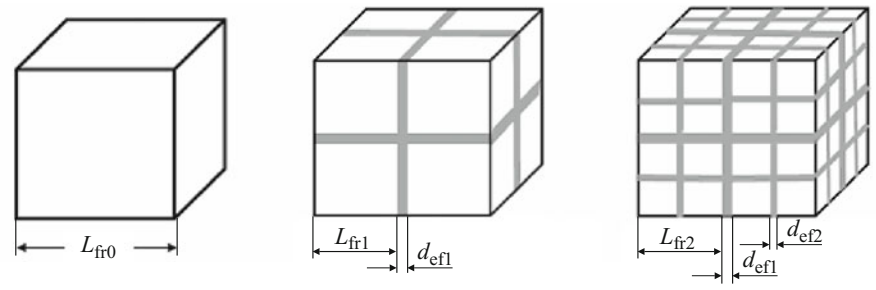

Fig. 1. Three-dimensional model of self-similar ensembles of crystals: *a*) initial phase; *b*) first generation; *c*) first and second generations.

The aim of the present work was to apply the model to estimating the resource of stored elastic energy in alloys undergoing martensitic transformation and characterized by the presence of a regular self-similar skeleton of martensite crystals and retained austenite.

METHODS OF STUDY

Let us recall the main concepts of the model. Figure 1 presents a three-dimensional variant where L_{fr0} specifies the starting value of parameter L.

The effective thickness d_{efj} of a crystal in each jth generation ($1 \le j \le n$) is expressed through the size of the bound domain $L_{b(j-1)}$ of the preceding generation by the relation

$$d_{efj} = \kappa d_j = \kappa \times 10^{-2} L_{fr(j-1)} = \chi L_{fr(j-1)},$$
$$\chi = \kappa \times 10^{-2}, \quad L_{frj} = \left[\frac{1-\chi}{2}\right]^j L_{fr0}. \qquad (2)$$

In Eq. (2) $1 \le \kappa \le 10^2$ and is independent of the index j numbering the generations, and $10^{-2} \le \chi < 1$. The values of $\kappa > 1$ are permissible because the shape of the crystals can be not only a thin-plate one but also a lenticular one, which contains not only a thin-plate regularly twinned central part (midrib) but also a large-volume enclosing "coat" that appears at a lower rate than the midrib. Alloys with shape memory effect (SME) commonly obey a variant with broadening of crystals during cooling.

In the jth generation the size of domain L_{frj} free of martensite crystals is lower than the initial size L_{fr0} by a factor of $\left[\frac{1-\chi}{2}\right]^j$. If the starting state of the austenite corresponds to a well-annealed single crystal with dislocation density $\rho \approx 10^4$ cm^{-2}, we have $L_{fr0} \approx 1/\sqrt{\rho} = 10^{-2}$ cm = 10^2 μm. At a specified L_{min} the number n of implemented generations meets the relation

$$n \le [\ln (L_{fr0}/L_{min})]/[\ln (2/(1-\chi)] \equiv n_{max}, \qquad (3)$$

in accordance with the inequality $L_{frn} \ge L_{min}$ and with Eq. (2), i.e., is equal to the integer part of the value of nmax. Closeness to a special concentration C^* is accompanied by growth in D_{cr}, and therefore the value of n will decrease at one an the same L_{fr0}.

When computing the fraction of the formed martensite δ_m, it is convenient to pass from dimensional L_{frj} and d_{efj} to dimensionless $\tilde{L}$ and $\tilde{d}$ by dividing them by L_{fr0} (at $\tilde{L}_{fr0} = 1$ and $0 < \tilde{L}_{frj} < 1$). With allowance for Eq. (2) the contribution of the jth generation of δ_{mj} can be expressed easily through χ, i.e.,

$$\delta_{mj} = 8^{(j-1)} \tilde{d}_{efj} [\tilde{d}^2_{efj} + 6\tilde{d}_{efj} \tilde{L}_{frj} + 12\tilde{L}^2_{frj}] =$$
$$= \chi(\chi^2 - 3\chi + 3)(1-\chi)^{3(j-1)}. \qquad (4)$$

It is obvious from the figure that the appearing structure is characterized by similarity coefficient $(1-\chi)/2$; upon formal transition to a limit $n \to \infty$ the fractal dimension of the austenite is

$$d_f = (\ln 8)[\ln (2/(1-\chi)]^{-1}, \quad 0 < d_f < 3. \qquad (5)$$

The maximum density of the elastic energy $(w_{elj})_m$ determining the value of the resource that can be accumulated in martensite crystals of the jth generation will be specified by relation

$$(w_{elj})_m = \frac{1}{2} G_m \varepsilon^2_{elj}. \qquad (6)$$

where G_m is the shear modulus in the martensite phase and ε_{elj} is the deformation limit of elasticity for the jth structural level. When evaluating ε_{elj} we base ourselves on the fact that the deformation limit of elasticity corresponds to the critical stress for generation of dislocations by Frank – Read sources. Then we may assume that

$$\varepsilon_{elj} = b_m / d_{efj}, \qquad (7)$$

where b_m is the Burgers vector, and the thickness d_{efj} naturally limits the maximum size of the working segments of the sources. Consequently, in accordance with Eqs. (4) – (7) the fractional contribution of the jth generation of crystals

TABLE 1. Reference Computational Values of n and $(\widetilde{W}_{el})_{\rm m}$ in the Three-Dimensional Model at $L_{\rm fr0} = 100$ μm

$(L_{\rm fr})_{\rm min}$, μm	$\chi = 0.01$		$\chi = 0.02$		$\chi = 0.1$		$\chi = 0.2$		$\chi = 0.3$	
	n	$(\widetilde{W}_{el})_{\rm m}$	n	$(\widetilde{W}_{el})_{\rm m}$	n	$(\widetilde{W}_{el})_{\rm m}$	n	$(\widetilde{W}_{el})_{\rm m}$	n	$(\widetilde{W}_{el})_{\rm m}$
0.02	12	$\mathbf{1.492 \times 10^9}$	11	1.691×10^8	10	3.811×10^6	9	1.951×10^5	8	1.532×10^4
0.036	11	3.768×10^8	11	1.691×10^8	9	1.059×10^6	8	6.097×10^4	7	5.468×10^3
0.36	8	6.068×10^6	7	7.161×10^5	7	8.167×10^4	6	5.949×10^3	5	693.92
3.6	4	2.457×10^4	4	1.184×10^4	4	1.740×10^3	3	1.762×10^2	3	84.972
34	1	2.970×10^2	1	1.470×10^2	1	27.10	1	12.2	1	7.3

$(W_{elj})_{\rm m}$ into the resource of elastic energy that can be accumulated by martensite in volume $(L_{\rm fr0})^3$ is equal to

$$(W_{elj})_{\rm i} = (w_{elj})_{\rm m}\delta_{{\rm m}j} = \frac{1}{2} G_{\rm m}\left[\frac{b_{\rm m}}{d_{{\rm ef}j}}\right]^2 \chi(\chi^2 - 3\chi + 3)(1-\chi)^{3(j-1)}. \quad (8)$$

Summing for all the permissible generations and allowing for Eqs. (2) and (8) we find

$$(W_{el})_{\rm m} = \sum_{j=1}^{n} (W_{elj})_{\rm m} = (W_{el})_0 \frac{(\chi^2 - 3\chi + 3)[4^n(1-\chi)^n - 1]}{\chi^{(3-4\chi)}},$$

$$(W_{el})_0 = \frac{1}{2} G_{\rm m}\left[\frac{b_{\rm m}}{L_{\rm fr0}}\right]^2. \quad (9)$$

It is obvious that at low $\chi \sim 10^{-2}$ and $n > 1$ formula (9) gives us a relation

$$(W_{el})_{\rm m} \approx (W_{el})_0 \frac{4^n}{\chi}, \quad (10)$$

which shows visually that the resource of elastic energy increases with respect to the starting value of $(W_{el})_0$ by a factor of $4n/\chi$. Clearly, the lower the value of $L_{\rm min}$ the greater, in accordance with (3), the number of generations n and hence the resource of elastic energy. Table 1 presents for illustration the values of reduced $(\widetilde{W}_{el})_{\rm m} = (W_{el})_{\rm m}/(W_{el})_0$ for different values of $L_{\rm min}$ and χ.

RESULTS

The results of the computation of n and $(\widetilde{W}_{el})_{\rm m}$ for four different values of $(L_{\rm fr})_{\rm min}$ at $L_{\rm fr0} = 10^2$ μm and five values of χ in the three-dimensional model are illustrated by Table 1. We include the values of 3.6 μm and especially of 34 μm as $(L_{\rm fr})_{\rm min}$ to reflect the possibility of getting close to the special concentration C^*, which is accompanied by growth in $D_{\rm cr}$.

The value of $(L_{\rm fr})_{\rm min} = 0.36$ μm = 36 nm exceeds the parameter of the fcc lattice of iron alloys by a factor of 100 and matches formally the geometrical limit of observation of condition (1), when the thin-plate component of a crystal has size d of the initially excited state in an elastic field of a dislocation, which is equal to the lattice parameter. The lower size $(L_{\rm fr})_{\rm min} = 20$ nm taken for comparison does not satisfy condition (1). However, this does not mean that such a choice has no physical meaning, because variants of twinning of the central part of a grain or of transformation of a grain as a whole are possible for grains of this small size [2, 4]. Then such a characteristic as crystal habit is eliminated, because the role of wave displacements responsible for formation of the habit is now played by the vibration modes of the grain as a whole. This makes it clear that only the boldfaced variant presented in the left top corner of Table 1 is physically unimplementable. It should also be noted that we have not taken into account the possibility of formation of transformation twins and mechanical twins when we performed summation in formula (9). If the twinning effect is allowed for, coarse crystals of the first generations can also have a level of the density of elastic energy comparable to that of small crystals of the last generations. However, then we should replace all values of $(W_{elj})_{\rm m}$ in expression (9) (for qualitative estimation of the upper boundary of the resource) by maximum $(W_{eln})_{\rm m}$ for the last generation (at $n = n_{\rm max} = 11$, $\chi = 0.01$) and remove them from the summation sign. Then the sum of the volume fractions of martensite of different generations will give us the total volume fraction of martensite; according to [2, 3] the latter in the given model is equal to

$$\delta_{\rm m} = \sum_{j=1}^{n} \delta_{{\rm m}j} = 1 - (1-\chi)^{3n}. \quad (11)$$

In the limiting case we obtain for $(W_{el})_{\rm m}$

$$(W_{el})_{\rm m} \approx \delta_{\rm i}(w_{eln})_{\rm m} = \frac{1}{2} G_{\rm m}\left[\frac{b_{\rm m}}{d_{{\rm ef}n}}\right]^2 \delta_{\rm i} = (W_{el})_0 \frac{4^{n-1}}{[1-\chi]^{2(n-1)}\chi^2}\delta_{\rm m}. \quad (12)$$

TABLE 2. Reference Computational Values of n and $(\tilde{W}_{el})_{\rm m}$ in the Three-Dimensional Model at $L_{\rm fr0} = 1$ μm

$(L_{\rm fr})_{\rm min}$, μm	$\chi = 0.01$		$\chi = 0.02$		$\chi = 0.1$		$\chi = 0.2$		$\chi = 0.3$	
	n	$(\tilde{W}_{el})_{\rm m}$	n	$(\tilde{W}_{el})_{\rm m}$	n	$(\tilde{W}_{el})_{\rm m}$	n	$(\tilde{W}_{el})_{\rm m}$	n	$(\tilde{W}_{el})_{\rm m}$
0.02	5	9.761×10^4	5	4.655×10^4	4	1.74×10^3	4	575.938	3	84.972
0.036	4	2.457×10^4	4	1.184×10^4	4	1.74×10^3	3	176.168	3	84.972
0.36	1	297.01	1	147.02	1	27.1	1	12.2	0	

Then at $n = 11$ and $\chi = 0.01$ we find from Eq. (12) that

$$(W_{el})_{\rm m} \sim (W_{el})_0 (36) \times 10^8. \quad (13)$$

Comparison with the data of Table 1 shows that the value of (13) is an order to magnitude higher than the maximum value found without allowance for the growth in the resource of accumulation of elastic energy in martensite crystals connected with twinning. Note that if we use the model to consider only thin-plate crystals, the fraction of retained austenite $\delta_{\rm A} = (1 - \chi)^{3n} \approx (0.99)^{33} \approx 0.718$ is high. The size of the free volumes of retained austenite after the appearance of 11 generations of martensite crystals is specified, according to (2), by the value $L_{{\rm fr}n} = [(1 - \chi)/2]^n L_{\rm fr0} = [0.99/2]^{11} L_{\rm fr0} \approx 4.37 \times 10^{-4} L_{\rm fr0}$.

Consequently, the contribution into the resource of elastic energy connected with retained austenite having no additional fine structure (for example, mechanical twins) is estimated as

$$(W_{el})_{\rm a} \approx \delta_{\rm m} (w_{eln})_{\rm a} = 1/2 G_{\rm A} [b_{\rm A}/L_{{\rm fr}n}]^2 \delta_{\rm A} \approx (W_{el})_0 \, 5.23 \times 10^6. \quad (14)$$

It is obvious that in the presence of fine structure in austenite, which allows us to use in (14) a value of $L_{{\rm fr}n}$ an oder of magnitude lower, we will obtain the same order of elastic energy as in equation (13). Twinning can be initiated in austenite by growth in the contribution of the interphase ("surface") energy into the energy resource. In the model considered the size of the surface of contact between martensite plates and austenite $S_{\rm am}$ after implementation of an nth generation is specified by expression

$$S_{\rm am} = 6 L_{{\rm fr}n}^2 8^n = 6(1 - \chi)/2]^{2n} L_{{\rm fr}n}^2 8^n = {\rm S02n}(1 - \chi)^{2n}, \quad S_0 = 6 L_{{\rm fr}n}^2. \quad (15)$$

At $n = 11$ and $\chi = 0.01$ we find from (15) that

$$S_{\rm am} \approx 0.80162048 S_0 \approx 1.64 \times 10^3 S_0.$$

Thus, our computations show that the resource of stored elastic energy in a structure with self-similar "skeleton" composed of twinned thin-plate martensite crystals, the spaces between which are filled with retained austenite, can be almost ten orders of magnitude higher that the starting resource $(W_{el})_0$. Since the elastic energy is squared with respect to the deformations, the deformation limit of elasticity increases by almost five orders of magnitude with respect to the starting value of $b_{\rm A}/L_{\rm fr0}$. For a typical Burgers vector in an fcc lattice of an iron alloy (with lattice parameter $a \approx 0.36$ nm) $b_{\rm A} = \frac{\sqrt{2}}{2} a \approx 0.25$ nm; then, for the chosen value of $L_{\rm fr0} = 100$ μm $+ 10^5$ nm the starting value is $\varepsilon_{el0} \approx (b_{\rm A}/L_{\rm fr0}) \approx 2.5 \times 10^{-6}$. Multiplying this value, in accordance with (13), by a factor 6×10^4, which reflects the change in the scale of the deformation elastic limit, we find $\varepsilon_{eln} \approx \varepsilon_{el11} \approx 0.15$. It should be noted that growth in $b_{\rm A}$ (for example due to transition to an ordered alloy) increases ε_{eln} proportionally. For example, if we choose $b_{\rm A} = a \approx 0.3$ nm, which corresponds to the lattice of phase B2 of titanium nickelide, we will obtain $\varepsilon_{eln} \approx 0.18$. Thus, the resource of elastic energy stored in MT (with participation of external deformation) is sufficient for recovery of strain at a level of about 10%. Then the participation of external deformation causing additional twinning of austenite and martensite can increase the resource of elastic energy and cause recovery of shape in the case of shape memory alloys, which is connected with the level of deformation exceeding the own strain of the transformation in spontaneous MT, as it has been observed for example, in [5, 6]. It is natural that in the case of the thermoelastic variant of formation of martensite, of comparatively low temperature ranges between the starts of forward and backward transformations and of relatively low changes in the specific volume, the degree of coherence of lattice junctions on all the possible boundaries is higher than for martensitic transformations with well manifested features of transition of the first kind. For this reason the possibility of an inverse order of displacements in such alloys is higher. It can be seen from Table 1 that the smallness of size $(L_{\rm fr})_{\rm min}$ is also important for high values of stored elastic energy.

It is clear that considerable lowering of the starting size $L_{\rm fr0}$ can suppress MT if the value of $(L_{\rm fr})_{\rm min}$ in the alloy is higher than $L_{\rm fr0}$. In the case of $L_{\rm fr0} > (L_{\rm fr})_{\rm min}$ the determined values of resource ε_{eln} preserve the order of magnitude though the number of generations n decreases and the starting value of ε_{el0} increases. For example, at $L_{\rm fr0} = 1$ μm, $\varepsilon_{el0} \approx (b_{\rm A}/L_{\rm fr0}) \approx 2.5 \times 10^{-4}$. It can be seen from Table 2

that the limiting variants for the evaluation should be $n = 4$ at $\chi = 0.01$ and $n = 5$ at $\chi = 0.02$.

For $n = 4$ at $\chi = 0.01$ we find from (12) that

$$(W_{el})_{\mathrm{m}} \approx (W_{el})_0(7.73) \times 10^4. \quad (16)$$

Then, in this case

$$\varepsilon_{eln} \approx \varepsilon_{el4} \approx \varepsilon_{el0}\sqrt{7.73} \times 10^2 \approx 2.5 \times 2.78 \times 10^{-2} \approx 7 \times 10^{-2},$$

i.e., is about twice lower than $\varepsilon_{el11} \approx 0.15$. For $n = 5$ at $\chi = 0.02$ we find from (12) that

$$(W_{el})_{\mathrm{m}} \approx (W_{el})_0(19.68) \times 10^4. \quad (17)$$

Then $\varepsilon_{eln} \approx \varepsilon_{el5} \approx \varepsilon_{el0}\sqrt{19.68} \times 10^2 \approx 2.5 \times 4.44 \times 10^{-2} \approx 0.11$, i.e., the estimate is closer to ε_{el11}.

DISCUSSION

Our computations have shown the following.

1. Recomputation of the estimated resource of stored elastic energy into the value of final strain is permissible for the case of shape memory alloys, where the energy of the external field providing the deformation of the shape is accumulated into elastic energy by ensembles of martensite crystals in a strictly determined (oriented and matched at all the structural levels) way. This makes it possible to recover the shape existing prior to the action of the deformation due to initiation of backward transformation during heating.

2. For simplicity, we have not taken into account the anisotropy of the shear modulus, which can be justified to some extent by the tendency to isotropy of the elastic properties arising closer to point M_s in SMA (as a rule, this is accompanied by softening of the modulus).

3. We have not taken into account the possibility of difference of the elastic modulus for different generations of crystals.

4. It is clear that when the value of recovered strain exceeds the own strain resource of the MT, we deal with additional elastic strain of the already transformed lattice.

5. Since the relaxation processes are not allowed for, the estimates obtained have a majorizing nature.

Despite the limitations mentioned, the consideration performed above seems to be physically transparent, visual, and simple mathematically. For this reason the relations obtained may be convenient for quantitative processing (in the first approximation) of experimental results.

CONCLUSIONS

By comparing generations of statistically similar ensembles of crystals to a symmetric set of self-similar generations of orthogonally conjugate crystals we can estimate the resource of elastic strain of the arising structures, which is useful for an analysis of observed recovered strain in shape memory alloys.

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