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Study of nonlinear deformatios of binary alloys with cubic structure

T. H. NGUYEN[a,b], C. GHEORGHIES[a*]
[a]*Faculty of Science - University Dunarea de Jos of Galati, Romania*
[b]*Faculty of Fundamental Science - University of Transport and Communications, Hanoi, Vietnam*

We have investigated the analytic expression for the strain-energy density of the binary alloys AB with b.c.c. and f.c.c. structure by the statistical moment method (SMM). The relation of the real stress σ_r and the strain ε for nonlinear deformed binary alloys are obtained. The influence of the temperature on the stress-strain curve and the maximum real stress σ_{rmax} of disorder alloys is investigated. The obtained results are applied to the V-0.10W, V-0.10Nb, V-0.10Ta, V-0.20Ta, Ta-0.10W, Ta-0.15W, Al-0.038Mg, Al-0.08Mg, Al-0.10Mg, Al-0.045Cu and Cu-0.10Zn alloys and compared with the experimental data.

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1. Introduction

Nonlinear deformation is one of the most important considerations in structure application of solid materials. Studies of temperature dependence for nonlinear deformed polymers, metals and alloys are presented by many researchers. In these works, the authors obtained the temperature dependence of elastic and nonlinear deformation by experimental and empirical methods; some of these studies are listed in Refs. 1-3. At high temperature regions, the stress σ depends strongly on the deformation rate $\dot{\varepsilon} = \frac{d\varepsilon}{dt}$, therefore, the equation of deformed state has the form $f(\sigma, \varepsilon, \dot{\sigma}, \dot{\varepsilon}, T) = 0$.

Since all these parameters of equation depend on temperature T, and formula for calculation of coefficients of equation depends not simply on these parameters. Therefore, the temperature dependence of the stress σ and the strain ε for nonlinear deformed metals and alloys can be found by experimental way [4]. The systems considered at high temperatures require the allowance for inharmonic effects. Influence of the thermal lattice expansion on the strain ε plays an important role and can not be neglected.

In this study, we present a new theoretical scheme on the nonlinear deformation of binary alloys based on the statistical moment method (SMM) [5, 6]. The analytic expression for the strain-energy density (SED) and the relation of the real stress σ_r and the strain ε for nonlinear deformed binary alloys are obtained. The inharmonic effects of lattice vibrations on the stress-strain curve and the maximum real stress σ_{rmax} of the alloys have also been studied. The SMM calculations are performed by using effective pair potentials for V-0.10W, V-0.10Nb, V-0.10Ta, V-0.20Ta, Ta-0.10W, Ta-0.15W alloys with body-centered cubic structure (b.c.c.) and Al-0.038Mg, Al-0.08Mg, Al-0.10Mg, Al-0.045Cu and Cu-0.10Zn alloys with face-centered cubic structure (f.c.c.) and compared with the experimental results.

2. Theoretical aspects

2.1 Free energy and the strain-energy density of binary alloys

Assume that an alloy AB has N atoms. C_A and C_B are the concentration of atoms A, B, respectively. Denote υ_a, υ_b the concentration of the lattice points of type a, b. The probability of atom α located in the lattice point a, b, is notated with p_α^a, p_α^b (α = A, B). Probabilities p_α^β (α = A, B; β = a, b) satisfy the following relations:
$p_A^a + p_B^a = 1;\ p_A^b + p_B^b = 1;\ \upsilon_a p_A^a + \upsilon_b p_A^b = C_A;\ \upsilon_a p_B^a + \upsilon_b p_B^b = C_B$.

Using the pair interactions and method of coordination spheres, the interaction energy of the binary alloys AB can be written as

$$U = \frac{N}{2}\sum_i [\upsilon_a p_A^a \varphi_{Ai}^a\left(|a_i + u_i|\right) + \upsilon_b p_A^b \varphi_{Ai}^b\left(|a_i + u_i|\right) + \upsilon_a p_B^a \varphi_{Bi}^a\left(|a_i + u_i|\right) + \upsilon_b p_B^b \varphi_{Bi}^b\left(|a_i + u_i|\right) = \sum_{\alpha,\beta} \upsilon_\beta p_\alpha^\beta u_\alpha^\beta \tag{1}$$

in which the quantities $u_\alpha^\beta = \frac{N}{2}\sum_i \varphi_{\alpha i}^\beta\left(|a_i + u_i|\right)$ have the form of the interaction potential energy of the N atoms system. The atoms chosen as base are atom α located in β point of the lattice. This system is called effective system (α, β). In eq. (1), $\varphi_{\alpha i}^\beta$ is the potential energy of interaction between particle i-th and the base particle; a_i is the vector determining the equilibrium position of particle i; u_i the displacement of i-th particle from it's equilibrium position. Thus the free energy of the system may be determined by the combination of the free energy of these effective system (α, β) as

$$F = \left(\upsilon_a p_A^a F_A^a + \upsilon_b p_A^b F_A^b + \upsilon_a p_B^a F_B^a + \upsilon_b p_B^b F_B^b\right) - TS = \sum_{\alpha,\beta} \upsilon_\beta p_\alpha^\beta F_\alpha^\beta - TS \tag{2}$$

where F_α^β is the free energy of the effective system (α, β) and S is the entropy of mixing

$$S = k_B \ln\left[\frac{(N_A + N_B)!}{N_A!N_B!}\right] \tag{3}$$

with k_B is the Boltzmann constant.

In order to define F_α^β we use the (SMM) described in [5,6]. The free energy of the effective system (α, β) will have form of the free energy of the systems of N harmonic oscillator [7]

$$F_\alpha^\beta = 3N\left\{\frac{u_{o\alpha}^\beta}{6} + k_B T\left[x_\alpha^\beta + \ln(1 - e^{-2x_\alpha^\beta})\right]\right\}, \tag{4}$$

with

$$x_\alpha^\beta = \frac{\hbar\omega_\alpha^\beta}{2k_B T} = \frac{\hbar}{2k_B T}\sqrt{k_\alpha^\beta / m^*}, \tag{5}$$

where $m^* = C_A m_A + C_B m_B$; m_A, m_B are the mass of atom A and B, and the sum of the effective pair interaction energies of the effective system (α, β), $u_{o\alpha}^\beta$, is given as

$$u_{o\alpha}^\beta = \sum_i \varphi_{\alpha i}^\beta\left(|a_i|\right). \tag{6}$$

In eq. (5), the second - order vibrational constant, k_α^β, is defined by

$$k_\alpha^\beta = \frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{\alpha i}^\beta}{\partial u_{ix}^2}\right)_{eq} \equiv m^*\left(\omega_\alpha^\beta\right)^2. \tag{7}$$

It is noted that when using eq. (4) the values of parameters $u_{o\alpha}^\beta$, k_α^β are taken at temperature T.

We study the nonlinear deformation of binary alloys in the condition of constant deformation rate. The strain-energy density (SED) has been used by Sih [8] and Nernat-Nassen [9] for the nonlinear deformation metals and alloys. The relation between the SED and the work density W^p has the form

$$\mathrm{SED} = \int_0^t \sigma_{ij}\,d\varepsilon_{ij} \approx W^p = \sigma_f \varepsilon^p,$$

where $\varepsilon^p = \left(\frac{2\varepsilon_{ij}^p\varepsilon_{ij}^p}{3}\right)^{1/2}$ for the proportional straining and σ_f is the flow stress or engineering ultimate stress.

In the present paper, the strain-energy density (SED) is given as

$$\mathrm{SED} = F^*(\varepsilon) - F^*(0) = C\sigma\varepsilon, \tag{8}$$

$$F^*(\varepsilon) = \frac{F(\varepsilon)}{V_{AB}(\varepsilon)},\ F^*(0) = \frac{F(0)}{V_{AB}}$$

where $F^*(0), F^*(\varepsilon)$ are the free energy of a volume unit of the binary alloy without deforming and with deforming by the external force p, respectively; C is the proportional coefficient deriving from the experimental data.

In the case of nonlinear deformation, the strain ε << 1, we can expand the free energy ψ(ε) as a power series of the strain ε

$$F(\varepsilon) = F(0) + \left(\frac{\partial F}{\partial\varepsilon}\right)_T\cdot\varepsilon + \frac{1}{2}\left(\frac{\partial^2 F}{\partial\varepsilon^2}\right)_T\cdot\varepsilon^2 + \ldots$$

If the truncate the above expansion up to the second-order terms, the free energy ψ(ε) has the form

$$F(\varepsilon) = F(0) + \left(\frac{\partial F(\varepsilon)}{\partial\varepsilon}\right)_T\cdot\varepsilon + \frac{1}{2}\left(\frac{\partial^2 F(\varepsilon)}{\partial\varepsilon^2}\right)_T\cdot\varepsilon^2. \tag{9}$$

Therefore, the strain-energy density (SED) of nonlinear deformed alloys is given as

$$f(\varepsilon) = SED = F(0)\left(\frac{1}{V_{AB}(\varepsilon)} - \frac{1}{V_{AB}}\right) + \frac{\varepsilon}{V_{AB}(\varepsilon)}\left(\frac{\partial F(\varepsilon)}{\partial\varepsilon}\right)_T + \frac{\varepsilon^2}{2V_{AB}(\varepsilon)}\left(\frac{\partial^2 F(\varepsilon)}{\partial\varepsilon^2}\right)_T \tag{10}$$

where $V_{AB}(\varepsilon) = Nv_{AB}(\varepsilon)$ and $v_{AB}(\varepsilon) = \frac{4}{3\sqrt{3}}a_{AB}^3(\varepsilon)$ and $v_{AB}(\varepsilon) = \frac{\sqrt{2}}{2}\mathbf{a}_{\mathbf{AB}}^3(\varepsilon)$ for a deformed alloy with b.c.c. structure and f.c.c. structure, respectively.

It noted that the nearest neighbor distance a_{AB} of binary alloys is given as [10]

$$a_{AB} = C_A a_A \frac{B_{T,A}}{\overline{B_T}} + C_B a_B \frac{B_{T,B}}{\overline{B_T}}, \tag{11}$$

where

$$\overline{B_T} = C_A B_{T,A} + C_B B_{T,B},$$

$$B_{T,\alpha} = \frac{\sqrt{3}}{4a_{\alpha}}\left\{\frac{1}{6}\left(\frac{\partial^2 u_{o\alpha}}{\partial a^2}\right)_T + \frac{\hbar\omega_{\alpha}}{4k_{\alpha}}\left[\left(\frac{\partial^2 k_{\alpha}}{\partial a^2}\right)_T - \frac{1}{2k_{\alpha}}\left(\frac{\partial k_{\alpha}}{\partial a}\right)_T^2\right]\right\}\left(\frac{a_{o\alpha}}{a_{\alpha}}\right)^3 \tag{12}$$

with $a_{o\alpha}$ (α = A, B) is the nearest neighbor distance at T = 0K of the pure metal α, a_{α} is the nearest neighbor distance at temperature T of the pure metal α, and the sum of the effective pair interaction energies of the pure metal α, $u_{o\alpha}$, is given as

$$u_{o\alpha} = \sum_i \varphi_{io}^{\alpha}\left(|a_i|\right). \tag{13}$$

In eq. (12) the second - order vibrational constant, k_{α}, is defined by

$$k_{\alpha} = \frac{1}{2}\sum_i \left(\frac{\partial^2 \varphi_{io}^{\alpha}}{\partial u_{ix}^2}\right)_{eq} \equiv m_{\alpha}^* \omega_{\alpha}^2, \tag{14}$$

where φ_{io}^{α} is the effective interaction energy between the zero-th and i-th atoms and u_i is the displacement of the i-th atom for the pure metal α.

The nearest neighbor distance $a_{AB}(\varepsilon)$ of binary deformed alloys has the form analogous (11)

$$a_{AB}(\varepsilon) = C_A a_A(\varepsilon)\frac{B_{T,A}(\varepsilon)}{\overline{B_T}(\varepsilon)} + C_B a_B(\varepsilon)\frac{B_{T,B}(\varepsilon)}{\overline{B_T}(\varepsilon)} \tag{15}$$

where $B_{T,\alpha}(\varepsilon)$, $\overline{B_T}(\varepsilon)$ have the form analogous (12), but the sum of the effective pair interaction energies, $u_{o\alpha}(\varepsilon)$, the second-order vibrational constants, $k_{\alpha}(\varepsilon)$, the vibrational frequencies, $\omega_{\alpha}(\varepsilon)$, depend on the strain ε.

The strain-energy density of the deformed alloys (10) can be written as

$$f(\varepsilon) = \left(\frac{1}{V_{AB}(\varepsilon)} - \frac{1}{V_{AB}}\right)\Psi(0) + \frac{\varepsilon}{V_{AB}(\varepsilon)}\left(\frac{\partial\Psi}{\partial a_{AB}}\right)_T\left(\frac{\partial a_{AB}}{\partial\varepsilon}\right)_T$$

$$+\frac{\varepsilon^2}{2V_{AB}(\varepsilon)}\left[\left(\frac{\partial^2\Psi}{\partial a_{AB}^2}\right)_T\left(\frac{\partial a_{AB}}{\partial\varepsilon}\right)_T^2 + \left(\frac{\partial\Psi}{\partial a_{AB}}\right)_T\left(\frac{\partial^2 a_{AB}}{\partial\varepsilon^2}\right)_T\right], \tag{16}$$

Where

$$\left(\frac{\partial\Psi}{\partial a_{AB}}\right)_T = \sum_{\alpha,\beta}\upsilon_{\beta}p_{\alpha}^{\beta}\left(\frac{\partial\Psi_{\alpha}^{\beta}}{\partial a_{AB}}\right)_T, \tag{17}$$

$$\left(\frac{\partial^2\Psi}{\partial a_{AB}^2}\right)_T = \sum_{\alpha,\beta}\upsilon_{\beta}p_{\alpha}^{\beta}\left(\frac{\partial^2\Psi_{\alpha}^{\beta}}{\partial a_{AB}^2}\right) \tag{18}$$

$$\left(\frac{\partial a_{AB}}{\partial\varepsilon}\right)_T \cong C_A\frac{B_{T,A}}{\overline{B_T}}\left(\frac{\partial a_A(\varepsilon)}{\partial\varepsilon}\right)_T + C_B\frac{B_{T,B}}{\overline{B_T}}\left(\frac{\partial a_B(\varepsilon)}{\partial\varepsilon}\right)_T,$$

$$\left(\frac{\partial^2 a_{AB}}{\partial\varepsilon^2}\right)_T \cong C_A\frac{B_{T,A}}{\overline{B_T}}\left(\frac{\partial^2 a_A(\varepsilon)}{\partial\varepsilon^2}\right)_T + C_B\frac{B_{T,B}}{\overline{B_T}}\left(\frac{\partial^2 a_B(\varepsilon)}{\partial\varepsilon^2}\right)_T \tag{19}$$

It is noted that the terms $\left(\frac{\partial a_{\alpha}}{\partial\varepsilon}\right)_T$ and $\left(\frac{\partial^2 a_{\alpha}}{\partial\varepsilon^2}\right)_T$ are given as

$$\left(\frac{\partial a_{\alpha}}{\partial\varepsilon}\right)_T = 2a_{o\alpha}(1+\varepsilon), \quad \left(\frac{\partial^2 a_{\alpha}}{\partial\varepsilon^2}\right)_T = 2a_{o\alpha}. \tag{20}$$

With the aid of eq. (4) the expression of the terms $\left(\frac{\partial F_{\alpha}^{\beta}}{\partial a}\right)_T, \left(\frac{\partial^2 F_{\alpha}^{\beta}}{\partial a^2}\right)_T$ in the eqs. (17) and (18) are determined in the form

$$\left(\frac{\partial F_{\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}}\right)_T = \frac{1}{2}\left(\frac{\partial u_{o\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}}\right)_T + 3\theta x_{\alpha}^{\beta}\coth x_{\alpha}^{\beta}\frac{1}{2k_{\alpha}^{\beta}(\varepsilon)}\left(\frac{\partial k_{\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}}\right)_T, \tag{21}$$

$$\left(\frac{\partial^2 F_{\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}^2}\right)_T = \frac{1}{2}\left(\frac{\partial^2 u_{o\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}^2}\right)_T + \frac{3\hbar\omega_{\alpha}^{\beta}}{4k_{\alpha}^{\beta}(\varepsilon)}\left[\left(\frac{\partial^2 k_{\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}^2}\right)_T - \frac{1}{2k_{\alpha}^{\beta}(\varepsilon)}\left(\frac{\partial k_{\alpha}^{\beta}(\varepsilon)}{\partial a_{AB}}\right)_T^2\right]. \tag{22}$$

From eqs. (16), (17), (18), (19) and (20) we obtain the expression of the SED

$$f(\varepsilon) = \left(\frac{1}{V_{AB}(\varepsilon)} - \frac{1}{V_{AB}}\right)\left[\sum_{\alpha,\beta}\upsilon_{\beta}p_{\alpha}^{\beta}F_{\alpha}^{\beta} - TS\right] + \frac{\varepsilon(1+\varepsilon)}{V_{AB}(\varepsilon)}\sum_{\alpha}C_{\alpha}\frac{B_{T,\alpha}}{\overline{B_T}}2a_{o\alpha}\sum_{\alpha,\beta}\upsilon_{\beta}p_{\alpha}^{\beta}\left(\frac{\partial F_{\alpha}^{\beta}}{\partial a_{AB}}\right)_T +$$

$$+\frac{\varepsilon^2}{2V_{AB}(\varepsilon)}\left\{\sum_{\alpha,\beta}\upsilon_{\beta}p_{\alpha}^{\beta}\left(\frac{\partial^2 F_{\alpha}^{\beta}}{\partial a_{AB}^2}\right)_T\left[(1+\varepsilon)\sum_{\alpha}C_{\alpha}\frac{B_{T,\alpha}}{\overline{B_T}}2a_{o\alpha}\right]^2 + \sum_{\alpha,\beta}\upsilon_{\beta}p_{\alpha}^{\beta}\left(\frac{\partial F_{\alpha}^{\beta}}{\partial a_{AB}}\right)_T\sum_{\alpha}C_{\alpha}\frac{B_{T,\alpha}}{\overline{B_T}}2a_{o\alpha}\right\}. \tag{23}$$

In the cases of disorder alloys AB with very small component B ($C_B << C_A$) we have [7]

$$p_A^a = p_A^b = C_A, \quad p_B^a = p_B^b = C_B,$$

$$F_A^a = F_A^b = F_A, \quad F_B^a = F_B^b = F_B.$$

By replacing these values in (2) we can find the free energy of system

$$F = \left(\upsilon_a p_A^a + \upsilon_b p_A^b\right)F_A + \left(\upsilon_a p_B^a + \upsilon_b p_B^b\right)F_B - TS$$

$$= C_A F_A + C_B F_B - TS = N_A F_A^* + N_B F_B^* - TS, \tag{24}$$

here F_A^*, F_B^* is the free energy of atom A and atom B surrounded by atoms A on the two first and second coordination spheres.

From eqs. (23), (24) we obtain the expression of the strain energy density of disorder alloys

$$f(\varepsilon) = \left(\frac{1}{V_{AB}(\varepsilon)} - \frac{1}{V_{AB}}\right)\left(\sum_{\alpha}C_{\alpha}F_{\alpha} - TS\right) + \frac{\varepsilon(1+\varepsilon)}{V_{AB}(\varepsilon)}\sum_{\alpha}C_{\alpha}\frac{B_{T,\alpha}}{\overline{B_T}}2a_{o\alpha}\sum_{\alpha}C_{\alpha}\left(\frac{\partial F_{\alpha}}{\partial a_{AB}}\right)_T +$$

$$+\frac{\varepsilon^2}{2V_{AB}(\varepsilon)}\left\{\sum_{\alpha}C_{\alpha}\left(\frac{\partial^2 F_{\alpha}}{\partial a_{AB}^2}\right)_T\left[(1+\varepsilon)\sum_{\alpha}C_{\alpha}\frac{B_{T,\alpha}}{\overline{B_T}}2a_{o\alpha}\right]^2 + \sum_{\alpha}C_{\alpha}\left(\frac{\partial F_{\alpha}}{\partial a_{AB}}\right)_T\sum_{\alpha}C_{\alpha}\frac{B_{T,\alpha}}{\overline{B_T}}2a_{o\alpha}\right\}. \tag{25}$$

2.2 Stress-strain relation for the nonlinear deformed binary alloys

For the nonlinear deformed binary alloys, we present the dependence of the stress σ on the strain ε as

$$\sigma = \sigma_0 \cdot \varepsilon^{\gamma} \tag{26}$$

with σ_0 and γ are constants for a given alloy. It is noted that the relation between the real stress σ_r appearing in the deformed sample and the stress on an area unit of sample σ is

$$\sigma_r = \frac{\sigma}{1+\varepsilon} \ . \tag{27}$$

Since the strain ε_p corresponding to the maximum real stress $\sigma_{r\max}$ is determined by

$$\frac{\partial \sigma_r}{\partial \varepsilon} = 0$$

using eqs. (26) and (27) one can find the following relations

$$\varepsilon_p = \frac{\gamma}{1-\gamma} \ , \tag{28}$$

$$\sigma_{r\max} = \sigma_o \frac{\varepsilon_p^{\gamma}}{1+\varepsilon_p} \ . \tag{29}$$

On the other hand, from eqs. (8), (25) we realize that $f(\varepsilon)$ is a function achieving the maximum value at the strain ε_p

$$f(\varepsilon_p) = f_{\max} = C\,\sigma_{\max}\varepsilon_p \ .$$

Therefore, we can easy obtain the maximum value of the stress $\sigma_{\max}$ as

$$\sigma_{\max} = \frac{f_{\max}}{C\varepsilon_p} \ . \tag{30}$$

From eqs. (27) and (30) the maximum real stress $\sigma_{r\max}$ is given as

$$\sigma_{r\max} = \frac{\sigma_{\max}}{1+\varepsilon_p} = \frac{f_{\max}}{C\varepsilon_p(1+\varepsilon_p)} \ . \tag{31}$$

In eq. (31), C is a proportionality coefficient and determined from eq. (8) and the experimental value of the stress $\sigma_{0.2}$ for a given alloy as

$$C = \frac{f(\varepsilon_{0.2})}{\sigma_{0.2} . \varepsilon_{0.2}} \ , \tag{32}$$

where the strain $\varepsilon_{0.2}$ = 0.2 % corresponding to the stress $\sigma_{0.2}$.

From eqs.(29), (31) and (32), it is easy to obtain the expression of the constant σ_o as

$$\sigma_o = \frac{f_{\max}}{f(\varepsilon_{0.2})} . \frac{\sigma_{0.2}\ \varepsilon_{0.2}}{\varepsilon_p^{\gamma+1}} \ . \tag{33}$$

Using eq. (25), one can find the strain ε_p corresponding to the maximum value of the strain-energy density $f_{\max} = f(\varepsilon_p)$ for disorder binary alloys. With the aid of eqs. (28) and (33), the values of the γ and σ_o constants are obtained. Therefore, the dependence of the stress σ on the strain ε (26) for nonlinear deformed disorder alloys is calculated.

3. Numerical results for disorder binary alloys with cubic structure

Table 1 summarizes the experimental data of potential parameters for b.c.c. and f.c.c. metals. The pair interaction potentials between two atoms of pure metal α is given as

$$\varphi^{\alpha}(r) = \frac{D}{n-m}\left\{ m\left(\frac{r_0}{r}\right)^{n} - n\left(\frac{r_0}{r}\right)^{m} \right\} . \tag{34}$$

$\varphi^{\alpha\alpha'}$ denotes the potential energy of interaction between two atoms α and α' (α, α' = A, B). In order to apply the theoretical calculation presented in the section 2, we used the following approximation

$$\varphi^{\alpha\alpha'} = \left(\varphi^{\alpha} + \varphi^{\alpha'}\right)/2 \ .$$

The dependence of the real stress σ_r on the strain ε for the nonlinear deformation process of disorder alloys is calculated. These results are presented in Fig. 1.

In Tables 2, 3 and 4 we compare SMM calculated results of $\sigma_{1\max}$ for the b.c.c. alloys and the f.c.c. alloys with the experimental data. The present SMM calculations of the maximum real stress $\sigma_{r\max}$ at various temperatures T agree with experimental values. Tables 2, 3 and 4 show that $\sigma_{r\max}$ and the strain ε_p corresponding to $\sigma_{r\max}$ as a function of the temperature T. We have found that the stress $\sigma_{r\max}$ and the strain ε_p depend strongly on the temperature T. The decrease of the real stress σ_r with increasing temperature arises from the thermal lattice expansion and the inharmonic effects are included through the explicit volume dependence of the vibrational frequency and the temperature dependence of the free energy.

In conclusion we have given out the analytic formula for the strain-energy density (SED), the stress-strain relation and the maximum real stress $\sigma_{r\max}$ for nonlinear deformed disorder alloys. The SMM calculations are performed by using effective pair potentials for V-0.10W, V-0.10Nb, V-0.10Ta, V-0.20Ta, Ta-0.10W, Ta-0.15W, Al-0.038Mg, Al-0.08Mg, Al-0.10Mg, Al-0.045Cu and Cu-0.10Zn alloys. In general, we have obtained good agreement in the maximum real stress $\sigma_{r\max}$ between our theoretical calculations and experimental values.

Table 1. Experimental values of potential parameters n, m, D and r_o for metals [11].

Metals	n	m	r_o (Å)	D/k_B (K)
W	10.5	7.0	2.7365	11278.8
Ta	11.0	6.0	2.8648	8508.1
Nb	8.5	5.0	2.8648	8307.3
V	14.0	9.5	2.6055	5782.6
Al	12.5	5.5	2.8541	2995.6
Mg	14.0	4.5	3.1882	1499.3
Cu	11.0	5.5	2.5487	3401.1
Zn	10.0	5.5	2.7622	1681.5

Table 2. SMM calculation results and experimental values [12] of $\sigma_{r\max}$ (in 10^8 Pa) and the strain ε_p (in %) at various temperatures for Ta-based (b.c.c.) alloys.

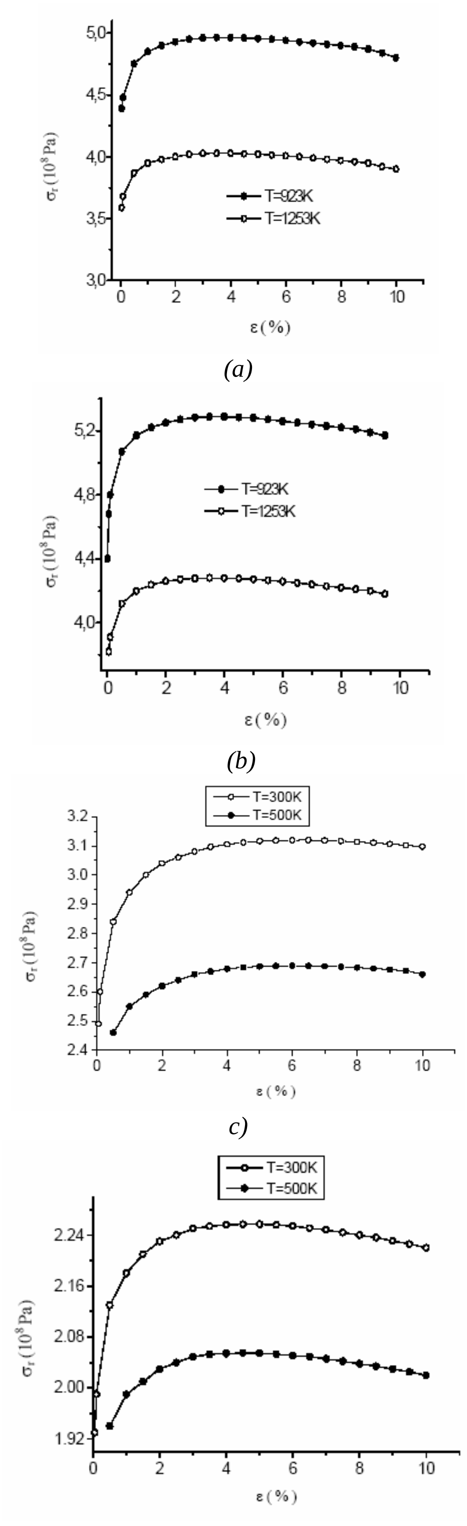
Alloys	T=1083K			T=1473K			T=1643K			T=1923K		
	ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$	
		SMM	**Exp.**		**SMM**	**Exp.**		**SMM**	**Exp.**		**SMM**	**Exp.**
Ta-0.10W	5.6	9.69	7.07	---	---	---	5.1	1.83	1.52	4.0	1.14	0.82
Ta-0.15W	---	---	---	4.3	3.36	3.25	---	---	---	---	---	---
Ta-0.20W	---	---	---	5.2	4.19	3.40	---	---	---	---	---	---

Table 3. SMM calculation results and experimental values [12] of $\sigma_{r\max}$ (in 10^8 Pa) and the strain ε_p (in %) at various temperatures for V-based (b.c.c.) alloys.

Alloys	T=293K			T=923K			T=1253K		
	ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$	
		SMM	**Exp.**		**SMM**	**Exp.**		**SMM**	**Exp.**
V-0.10W	4.2	6.62	5.39	3.8	4.94	2.55	3.6	4.01	1.25
V-0.10Nb	4.2	7.13	6.28	3.8	5.27	5.39	3.6	4.27	2.55
V-0.20Nb	4.3	7.92	7.36	3.9	5.69	5.59	3.7	4.48	3.82
V-0.10Ta	4.2	7.11	6.08	3.8	5.09	3.63	----	----	----
V-0.20Ta	4.3	6.31	7.06	3.9	4.30	4.41	----	----	----

Table 4. SMM calculation results and experimental values [13] of $\sigma_{r\max}$ (in 10^8 Pa) and the strain ε_p (in %) at various temperatures for Al-based (f.c.c.) alloys.

Alloys	T=300K			T=500K			T=700K		
	ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$		ε_p	$\sigma_{r\max}$	
		SMM	**Exp.**		**SMM**	**Exp.**		**SMM**	**Exp.**
Al-0.038Mg	6.1	1.57	1.86	5.8	1.41	-----	5.5	1.27	-----
Al-0.08Mg	6.2	2.61	2.89	5.9	2.32	-----	5.7	2.02	-----
Al-0.10Mg	6.2	3.12	3.17	6.0	2.69	-----	5.7	2.39	-----
Al-0.045Cu	4.6	2.26	2.20	4.5	2.06	-----	4.3	1.92	-----



(a)

(b)

c)

d)

Fig.1. The dependence of stress σ_l on the strain ε for nonlinear deformed disorder alloys at various temperatures T: (a) V-0.10W alloy; (b) V-0.10Nb alloy; (c) Al-0.01Mg alloy and (d) Al-0.045Cu alloy.

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[*] Corresponding author: c.gheorghies@ugal.ro