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Modulus of Elasticity of Lab_6 - Meb_2 (Me - Ti, Zr, Hf) Composite at High Temperatures based on the Interfacial Interactions

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I. Introduction

A quasi-binary eutectic composite is a system of two components in the absence of their mutual solubility. In eutectic systems, the boundary contact between the components may be coherent, semicoherent or amorphous depending on the types and structures ratio parameters of their crystal lattices.

If you know the general principle of calculating of the theoretical strength under uniaxial tension through the energy of pure components, the problem of the same calculation for composite is rather ambiguous and complex, which is associated with the influence of the boundaries of the components.

This paper discusses the mechanical properties such as strength, elastic modulus, maximum strain, as well as the surface energy of components contacts in composite as a function of temperature. All of these characteristics are determined by the energy of interaction between the elements in composite. The object of study is Quasi-binary eutectic composites LaB_6 –MeB_2 (Me - Ti, Zr, Hf). Mutual insolubility components of these systems is confirmed by quantum-mechanical calculations and is presented in [1].

II. Research Methods, Numerical Simulation and Discussion of Results

The method of determining the total energy of the alloy per molecule within the pseudopotential method is based on the summation of the potentials of paired intermolecular interactions [2]. If the concentration of component A is denoted C, the energy of system from two components can be written

$$U = U_{AA}C^2 + U_{BB}(1-C)^2 + 2C(1-C)U_{AB}. \quad (1)$$

Here

$$U_{AA}C^2 = \frac{1}{2N}\sum_{i\neq j}\Phi_{AA}(R_{ij}), \quad (2)$$

$$U_{BB}(1-C)^2 = \frac{1}{2N}\sum_{i\neq j}\Phi_{BB}(R_{ij}), \quad (3)$$

$$U_{AB}\cdot 2C(1-C) = \frac{1}{2N}\sum_{i\neq j}\Phi_{AB}(R_{ij}), \quad (4)$$

where Φ_{AA}, Φ_{BB}, Φ_{AB} - potentials of interactions between these components [2], and U_{AA}, U_{BB}, U_{AB} - the energy of interaction between the components A- A, B – B and A -B.

The first component has a connection of A - A type, and the second component connection B - B, at the interface - only A - B connection. Equation (1) can be written as

$$U = U_{AA}C^2 + U_{BB}(1-C)^2 + 2C(1-C)U_{AB} = C^2U^*_{AA} + (1-C)^2U^*_{BB}, \quad (5)$$

where

$$U^*_{AA} = U_{AA} + U_{AB}\frac{1-C}{C}, \; U^*_{BB} = +U_{BB} + U_{AB}\frac{C}{1-C}. \quad (6)$$

Tension along the z axis is determined from the relation [3]

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$$\sigma_z = \frac{1}{S_i \cdot d} \cdot \frac{\partial U_{ii}(d)}{\cdot \partial e_z}, \qquad (7)$$

where e_z - relative deformation, and U_{ii} is a U_{AA} or U_{BB}, d - lattice parameter in the direction of the axis of deformation, S_i - atomic plane area in a crystal lattice that is perpendicular to the axis of strain. For calculating the formulas based on strength (6, 7) there is the following relationship:

$$\sigma_A^* = \left[\frac{1}{d_A \cdot S_A} \frac{\partial U_{AA}(d_A)}{\partial e_z} + \frac{1-C}{C} \frac{1}{d_V \cdot S_V} \frac{\partial U_{AB}(d_V)}{\partial e_z} \right] = \sigma_A + \frac{1-C}{C} \sigma_{AB}, \qquad (8)$$

$$\sigma_B^* = \left[\frac{1}{d_B \cdot S_B} \frac{\partial U_{BB}(d_B)}{\partial e_z} + \frac{C}{1-C} \frac{1}{d_V \cdot S_V} \frac{\partial U_{AB}(d_V)}{\partial e_z} \right] = \sigma_B + \frac{C}{1-C} \sigma_{AB} \qquad (9)$$

The paper considers in equal deformed state condition in which the permissible deformation of the composite in tension coincides with the maximum deformation of the reinforcing fibers. In equal deformed state, according to the rule of mixtures, excluding the impact of joining the borders of the two components, the maximum strength of the quasi-binary system will be

$$(\sigma_C)_{\max} = \delta\Omega_A \cdot \sigma_A + \delta\Omega_B \cdot \sigma_B^{\max}. \qquad (10)$$

Here, $\delta\Omega_A$, $\delta\Omega_B$ the volume fractions of LaB_6 and MeB_2, $\sigma_B^{\max}$ - maximum strength of MeB_2 and σ_A – strength of LaB_6 or resistance of the matrix at the maximum deformation of hardener (i.e. when $\varepsilon = \varepsilon_{\max}$), which is called "temporary resistance."

With the impact of borders joining have

$$(\sigma_C^*)_{\max} = \delta\Omega_A \cdot \sigma_A^* + \delta\Omega_B \cdot \sigma_B^{*(\max)}. \qquad (11)$$

With a very small strain the curve stress - strain is close to a linear law, and then:

$$\sigma_c = \delta\Omega_A\sigma_A + \delta\Omega_B\sigma_B = E_A\varepsilon_A\delta\Omega_A + E_B\varepsilon_B\delta\Omega_B, \qquad (12)$$

and taking into account the phase of interaction (Figure I.)

$$\sigma_c^* = \delta\Omega_A\sigma_A^* + \delta\Omega_B\sigma_B^* = E_A^*\varepsilon_A\delta\Omega_A + E_B^*\varepsilon_B\delta\Omega_B, \qquad (13)$$

where σ_c; σ_A; σ_B stresses in composite and in components A and B,

E_i, E_i^*, $\varepsilon_{i\,i}$ - elastic modulus and the strain of the components (and without taking into account the interfacial interaction).

In equal deformed state ($\varepsilon_c = \varepsilon_A = \varepsilon_B$)

$$E_c = \sigma_c / \varepsilon_c : \quad E_c^* = \sigma_c^* / \varepsilon_c \qquad (14)$$

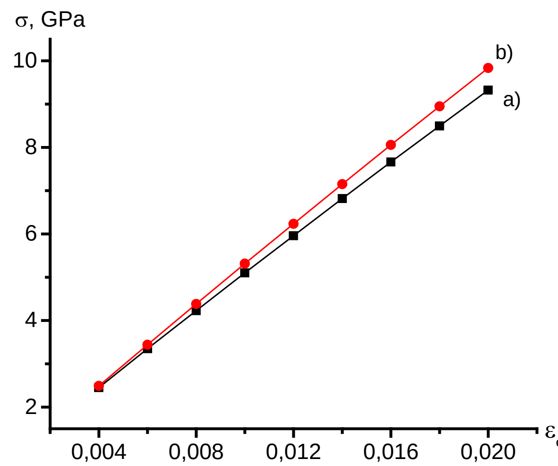

Fig. I: The linear dependence of the composite stress from small strain ε_c: $a)\ \sigma = \sigma_c$, $b)\ \sigma = \sigma_c^*$.

For small values of deformation the calculated values of the stress and the elastic modulus of LaB_6 - TiB_2 composite (at zero temperature) are shown (Table I.).

Table I: The calculated values of the stress and the average value of elastic modulus (in GPa) of LaB_6 - TiB_2 composite with and without interfacial interaction

ε_c	σ_c	σ_c^*	$\overline{E}_c$	$\overline{E}_c^*$
0,004	2,041	2,121	510	530
0,006	3,063	3,185		
0,008	4,081	4,252		
0,010	5,101	5,312		

To identify the mechanical characteristics depending on the temperature, it is necessary to be able to calculate the energy of the electron-ion system of the materials at different temperatures. In the method of pseudopotentials, it means to find a change in the volume of the unit cells, at temperatures different from zero, ie, obtain the explicit dependence of the total energy of the lattice parameters and volume at nonzero temperature.

Note that the calculation of the energy of the electron - ion system in the second-order of perturbation theory in the pseudopotential means using the harmonic approximation. But application of this approach in the lattice dynamics enough to calculate certain physical characteristics that are associated with a change in crystal lattice volume with increasing temperature. This problem can be avoided if use [5] "quasi-harmonic model" (developed by the authors), which allows to identify the temperature dependence of the unit cell volume in the harmonic approximation. The result is a dependence of the energy of the electron-ion system on temperature through the unit cell volume

$$U_{i,j}(T)=U_{i,j}(\Omega_{i,j}(T)) \qquad (15)$$

The final formula for calculating the theoretical strength at uniaxial tensile versus temperature are presented in the form:

$$\sigma_A^*(T)=\sigma_A(T)+\frac{1-C}{C}\sigma_{AB}(T); \quad \sigma_B^*(T)=\sigma_B(T)+\frac{1-C}{C}\sigma_{AB}(T) \ . \qquad (16)$$

In borides with a high content of boron, the boron atoms form stable complexes structuras (B_6), their influence on the physico-mechanical characteristics of the material occurs at high temperatures, which leads to the appearance of peaks or abrupt changes in the physical and mechanical characteristics [6].

It was found that for uniaxial deformation in the temperature range from 0 to 2750 K the characteristic exponential dependence of strength on temperature disrupted in a temperature range (1300 - 2200K) in the case of LaB_6. In this interval an increase in temperature leads to higher theoretical strength. The same dependence is observed for eutectic systems LaB_6 – MeB_2 (Me - Ti, Zr, Hf), which constitutes mainly from the LaB_6 [1].

Accounting for the interaction energy between heterogeneous elements A and B at the interface of the two phases results in a change of its value and the maximum deformation and hence the maximum strength in the composite. Note that at T = 0K for MeB_2 maximum deformation (Me -Ti, Zr, Hf) is approximately $\varepsilon_{\max} \approx 0,099$ [6]. In the calculation of the effective strength the extension member results in an increase of maximum deformation (at T = 0 K $\varepsilon^*_{B\max}=0.11$, and $\varepsilon^*_{B\max}=0.1161$ for in case of TiB2 and ZrB2, for HfB2 $\varepsilon^*_{B\max}=0.1158$. The increase in the maximum deformation of hardener - the result of interactions of the components (phases), which entails an increase in the temporary matrix resistance, tending to its maximum value, and, in general, increases the strength of the composite.

Results of computational experiment on the calculation of the elastic modulus for composite and components, as well as their temperature dependence are presented in Table. II-III.

Table. II: The elastic moduli of composite materials and components in the system LaB_6 – MeB_2 and experimental value in Gpa

Phase	*E* (Calculation)	*E* (Experiment)	
LaB_6	495,05	478,73 [7]	320 [9]
TiB_2	600,06	540,53 [7]	545[9]
HfB_2	523,97	479,71 [7]	
ZrB_2	534,67	495,80 [8]	430[9]
LaB_6 - TiB_2	506,28	-	
LaB_6 - HfB_2	507,63	-	
LaB_6 - ZrB_2	507,46	-	430-450[9]

The values obtained for the Young's modulus are close to their experimental values within acceptable limits (the maximum relative error of ~ 7%), given that the calculations considered only perfect single crystals, real crystals always have a lower value.

Table III: Dependence of the Young's modulus (GPa) of components LaB_6, TiB_2 and composite LaB_6 – TiB_2 on temperature

T, K	E_A	E_B	E_c
0	495,05	600,06	506,28
300	487,50	593,35	498,86
500	478,19	580,28	489,11
750	466,25	571,09	477,41
1000	450,76	548,67	461.24
1500	430,09	530,29	440,81
2000	400,15	500,07	410,84
2500	360,23	476,13	372,63
2750	330,18	440,06	341,94

If a crystal is subjected to deformation and simultaneously the temperature rises, then in parallel with deformation thermal expansion will operate. Quantum-mechanical calculations show that the interaction between the boron atoms is much stronger than between metal and boron, and even more than metal-metal bond [2]; i.e. B_6 complex expansion requires higher temperatures. This is confirmed by results of calculating the dependence of deformation on the temperature.

At temperatures T> 1300 K expansion of B_6 complex on the plane [200] counteracts the uniaxial strain (stretch) of the complex in the perpendicular direction, as a result of which there appear anomalies in the graph of the strength – temperature dependence. At relatively small deformations, in which the elastic modulus is determined, this effect is not observed (Figure II). Figure III shows the dependence of the modulus of elasticity- maximum strength ratio of the composite on the temperature. In the temperature range of 1000-2500 K, an area of the characteristic hardening of a composite is marked out.

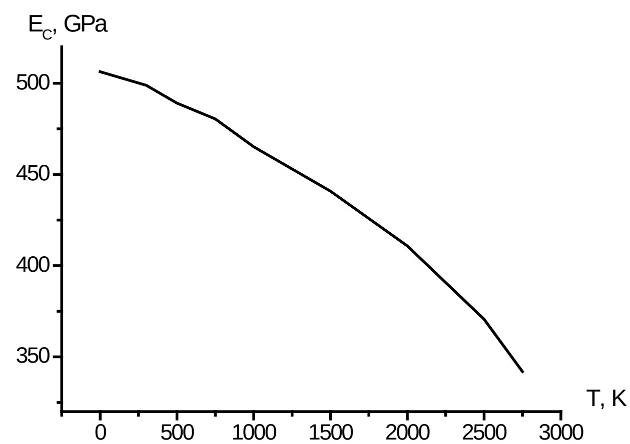

Fig. II: The dependence of the elastic modulus on temperature of the LaB_6 – MeB_2 composite

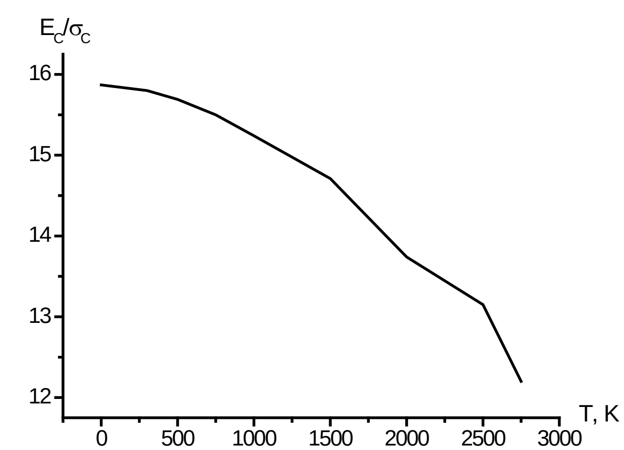

Fig. III: Temperature dependence of the ratio of the modulus of elasticity and ultimate strength of the LaB_6 – MeB_2 composite

Accounting components interaction in composites at the interface connections increases the value of composite modulus of elasticity.

The boundary of the two phases in the composite serves as a redistribution of property area: increasing the plasticity of refractory component and the theoretical strength and elastic modules of the composite as a whole. Up to the melting temperature composites LaB_6 – MeB_2 have high strength and elastic modulus.

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