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# The Temperature Dependences of Elastic Modulus of Composites $\text{LaB}_6\text{-MeB}_2$



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## Abstract

Mechanical properties of a composite have been calculated within the pseudo potential method. At calculating the system energy we have taken into account non-harmonic effects, connected with thermal vibrations of atoms, using the quasi-harmonic approximation. For equally deformed states we have obtained stress-strain dependence. We have calculated elastic modulus, maximum strain and the corresponding maximum strength for  $\text{LaB}_6\text{-MeB}_2$  composite with eutectic composition with regard to the influence of the components' boundaries, as well as their temperature dependence. There is an exponential dependence of elastic modulus on the composite temperature and in the dependence of elastic modulus - maximum strength ratio on the temperature there is a section where the composite hardening at high temperatures is observed. Different changes in strength and modulus of elasticity depend on the ratio of elastic and total strain of the composite at high temperatures.

Accounting of interfacial interaction leads to an increase in the maximum strength of the composite in the whole temperature range, and that provides an increase in the modulus of elasticity.

**Keywords:** Eutectic; Interconnect borders; Strength composites; Elastic modulus; Deformation

## 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, semi coherent 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  $\text{LaB}_6\text{-MeB}_2$  ( $\text{Me-Ti, Zr, Hf}$ ). Mutual insolubility components of these systems are confirmed by quantum-mechanical calculations and are presented in [1].

## Research Methods, Numerical Simulation and Discussion of Results

The method of determining the total energy of the alloy per molecule within the pseudo potential 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,  $\Phi_{AA}$ ,  $\Phi_{BB}$ ,  $\Phi_{AB}$  - 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,

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

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

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

Where,  $e_z$  - relative deformation, and  $U_{ii}$  is a UAA or UBB,  $d$  - 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:

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

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

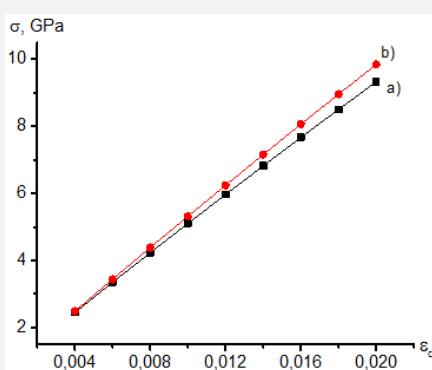
The paper considers in equal deformed state condition in which the permissible deformation of the composite in tension coincides with the maximum deformation of the reinforcing fibers. In equal deformed state, according to the rule of mixtures, excluding the impact of joining the borders of the two components,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

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

Here,  $\delta\Omega_A$ ,  $\delta\Omega_B$  the volume fractions of  $\text{LaB}_6$  and  $\text{MeB}_2$ ,  $\sigma_B^{\max}$  - maximum strength of  $\text{MeB}_2$  and  $\sigma_A$  - strength of  $\text{LaB}_6$  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

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



**Figure 1:** The linear dependence of the composite stress from small strain  $\varepsilon_c$ :

a)  $\sigma = \sigma_c$ , b)  $\sigma = \sigma_c^*$ .

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

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

and taking into account the phase of interaction (Figure 1)

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

Where,  $\sigma_c$ ;  $\sigma_A$ ;  $\sigma_B$  resses in composite and in components A and B,

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

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

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

For small values of deformation the calculated values of the stress and the elastic modulus of  $\text{LaB}_6\text{-TiB}_2$  composite (at zero temperature) are shown (Table I).

**Table 1:** The calculated values of the stress and the average value of elastic modulus (in GPa) of  $\text{LaB}_6\text{-TiB}_2$  composite with and without interfacial interaction,

$\varepsilon_c$	$\sigma_c$	$\sigma_c^*$	$\bar{E}_c$	$\bar{E}_c^*$
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 pseudo potentials, 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 pseudo potential means using the harmonic approximation. But application of this approaches 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

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

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

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

In borides with a high content of boron, the boron atoms form stable complexes structures ( $B_6$ ), 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 2750K 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  $\epsilon_{max} \approx 0,099$  [6]. In the calculation of the effective strength the extension member results in an increase of maximum deformation (at  $T = 0 K$   $\epsilon_{B,max}^* = 0.11$ , and  $\epsilon_{B,max}^* = 0.1161$  for in case of  $TiB_2$  and  $ZrB_2$ , for  $HfB_2$   $\epsilon_{B,max}^* = 0.1158$ ). 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 2 & 3. The values obtained for the elastic modulus are close to their experimental values within acceptable limits (the maximum relative error of <9%), given that the calculations considered only perfect single crystals, real crystals always have a lower value.

**Table 2:** The elastic modulus of composite materials and components in the system  $LaB_6$ - $MeB_2$  and experimental value in Gpa.

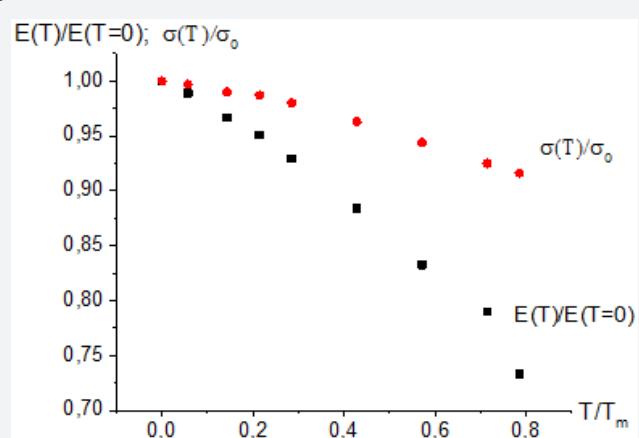
Components	E (T=298 K)		Composit	Ec (T=298 K)	
	Calculation	Experiment [7,8]		Calculation	Experiment [9]
$LaB_6$	489,64	487,73			
$ZrB_2$	523,86	495-430	$LaB_6$ - $ZrB_2$	506,56	430-450
$TiB_2$	590,08	550-540	$LaB_6$ - $TiB_2$	509,53	
$HfB_2$	520,87	479,71	$LaB_6$ - $HfB_2$	501,82	
$NbB_2$	547,56	540-450	$LaB_6$ - $NbB_2$	516,04	
$TaB_2$	695,08	686,7	$LaB_6$ - $TaB_2$	552,48	
$VB_2$	355,93	340	$LaB_6$ - $VB_2$	427,18	
$CrB_2$	476,87	450	$LaB_6$ - $CrB_2$	484,19	

**Table 3:** Dependence of the elastic modulus (GPa) of components  $LaB_6$ ,  $TiB_2$  and composite  $LaB_6$ - $TiB_2$  on temperature.

T,K	E <sub>A</sub>	E <sub>B</sub>	E <sub>c</sub>
0	492,05	600,02	506,28
300	488,50	589,85	489,86
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

Figure 2 shows the dependences of the relative values of the elastic modulus ( $E(T)/E(T=0)$ ) and the theoretical strength ( $\sigma(T)/\sigma(T=0)$ ) on the temperature for  $LaB_6$ . As the temperature rises, the  $LaB_6$  single crystal loses its elastic properties faster than strength. Figure 3 shows almost identical dependences of

the relative values of the elasticity modulus on the temperature for  $LaB_6$  and  $TiB_2$ . In both cases, the interval of temperature change is  $0 \leq T \leq 2750K$ ;  $E(T=0)$  and  $\sigma(T=0)$  is the value of the elastic modulus and strength at absolute zero temperature [7-9].



**Figure 2:** Dependences of the modulus of elasticity and strength on temperature for  $TiB_2$ .

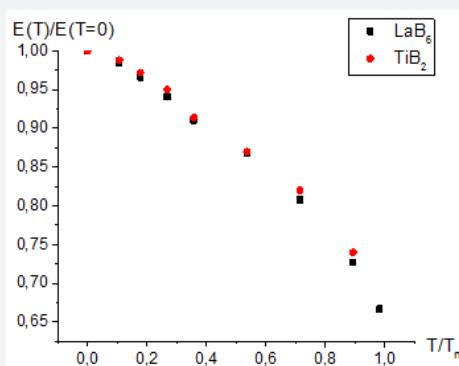


Figure 3: Dependence of the elastic moduli on temperature for  $\text{LaB}_6$  and  $\text{TiB}_2$ .

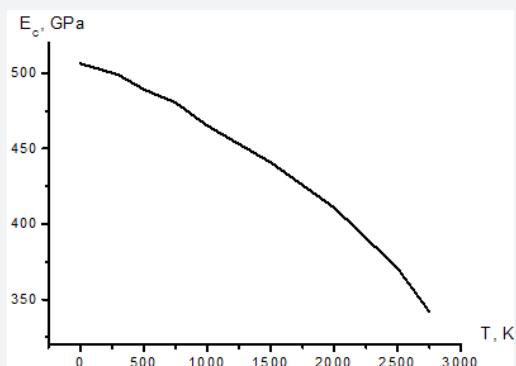


Figure 4: The dependence of the elastic modulus on temperature of the  $\text{LaB}_6\text{-MeB}_2$  composite.

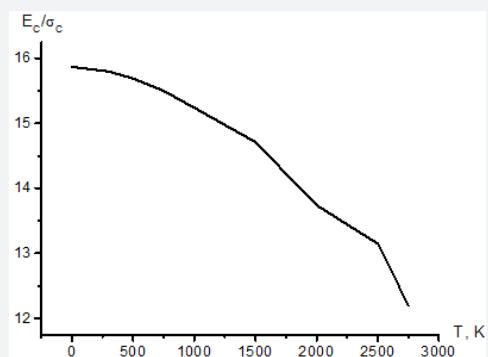


Figure 5: Temperature dependence of the ratio of the modulus of elasticity and ultimate strength of the  $\text{LaB}_6\text{-MeB}_2$  composite.

If a crystal is subjected to deformation and simultaneously the temperature rises, then in parallel with deformation thermal

expansion will operate. At temperatures  $T > 1300\text{K}$  expansion of  $\text{B}_6$  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 4 & 5) shows the dependence of the modulus of elasticity - maximum strength ratio of the composite on the temperature. In the temperature range of 1000-2500K, an area of the characteristic hardening of a composite is marked out.

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  $\text{LaB}_6\text{-MeB}_2$  have high strength and elastic modulus.

## References

- Zakaryan D, Kartuzov V, Khachatrian A, Sair A (2011) Calculation of composition in  $\text{LaB}_6\text{-TiB}_2$ ,  $\text{LaB}_6\text{-ZrB}_2$  eutectics by means of pseudopotential method, Journal of the European Ceramic Society 31(7): 1305-1308.
- Zakarian D, Khachatrian A (2013) Modeling of intermolecular interactions in the system  $\text{LaB}_6$  -  $\text{MeB}_2$  within the pseudo potential method, Reports of the National Academy of Science of Ukraine, Ukraine 1: 77-82.
- Zakarian D, Kartuzov V, Khachatrian A (2016) Prediction of the Mechanical Properties of  $\text{LaB}_6\text{-ZrB}_2$  Materials in View of the Effect of Their Intercomponent Boundaries, Strength of Materials 48(2): 290-293.
- Zakarian D (2014) Calculation of the surface contact of components in quasibinary eutectic systems, Reports of the National Academy of Sciences of Ukraine 11: 82-87.
- Zakarian D, Kartuzov V, Khachatrian A (2016) Quasi-harmonic approximation model in the theory of pseudopotentials, Reports of the National Academy of Sciences of Ukraine 4: 55-61.
- Zakarian D, Kartuzov V, Khachatrian A (2015) Theoretical Strength of Borides and Quasibinary Borid Eutectics at High Temperatures, Powder Metallurgy and Metal Ceramics 54(3): 210-214.
- Serebryakova TI, Neronov VA, Pekhov AD (1991) High borides. Metallurgy, Russia.
- Franzevich IN, Voronov FF, Bakuto SA (1982) Elastic Constants and modules of elasticity of metal and nonmetal. Naukova Dumka, Kiev.
- Lyashenko AB, Experimental determination of the modulus of elasticity-Private message (unpublished work) - Private message, Kiev-IPMS National Academy of Science, Ukraine.



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