УДК 535.323.341:546.261

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# MODELING OPTICAL PROPERTIES OF SiC + AlN TYPE HETEROPHASE CERAMIC MATERIALS BY THE MEANS BRUGGMAN THEORY

*Ceramic samples SiC and AIN as well as SiC samples with different quantity of AlN admixtures was studied by infrared reflection spectroscopy and spectroellipsometry. The numerical modeling of optical properties of SiC + AlN type ceramic materials was made using the Bruggman theory. The comparison of experimental spectra of refractive index and extinction coefficient for two-phases samples of SiC + AlN type with theoretical calculated spectra enable us conclude that the SiC + AlN system is heterophase eutectic mechanical mixture big clusters which are equally distributed in the space of the sample.*

The physical properties of silicon carbide and possibilities of its use in device design have been a subject of considerable interest in modern science. Ceramic materials are characterized by a composition of electrical, thermal and chemical properties, which make they very attractive for using in device application for modern technology. Strong chemical bonding and physical stability are favorable for development of devices, which work under great load and in the aggressive environment. SiC is very useful as a base of abrasive, heatproof, electrotechnical, wearproof materials that used in industrial application. New SiC ceramic materials are used as substitute for expensive refractory metals and alloys. There are many types of ceramic materials with different properties and phase structure. Most of those materials are heterophase composition of SiC with special admixtures. The admixtures differ from the main phase SiC in chemical and physical properties, and using that permits to obtain ceramic materials with proper physical and chemical properties. There are different controlling methods for chemical and phase structure of ceramic materials. Optical methods are fast and non-destructive examination methods. Studying of optical properties of ceramic materials gives possibility to made conclusion about phase structure. The optical properties of ceramic SiC with AlN admixtures are considered in this article. Several ceramic samples SiC and AlN as well as SiC samples with different quantity of AlN admixtures was studied by infrared reflection spectroscopy and spectroellipsometry in the visible and ultraviolet region.

## 1. Bruggman effective-medium approximation

The Bruggman theory [1] is a good method for investigating and modeling the heterophase structures. Bruggman effective-medium approximation model gives one dielectric constants for different types of physical mixtures: homogeneous mixtures of spheres, spherical inclusion of a second component embedded in a matrix, mixtures of lamellar with a given or random orientation lamellar inclusion, etc.

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The effective dielectric constant ε of the physical mixture is described by the following equation:

$$(1-c)\frac{\varepsilon_1-\varepsilon}{\varepsilon_1+2\varepsilon}=c\frac{\varepsilon-\varepsilon_2}{\varepsilon_2+2\varepsilon}. \quad (1)$$

Were $c$ is the concentration of the admixtures with complex dielectric constant Є2 in matrix with complex dielectric constant ει. For $c = 0$, $\varepsilon = \varepsilon 1$, and $c = 1, \varepsilon = \varepsilon 2$· Equation (1) works out as

$$2\varepsilon^2-\left[(3c-1)(\varepsilon_2-\varepsilon_1)+\varepsilon_1\right]\varepsilon-\varepsilon_1\varepsilon_2=0. \quad (2)$$

In general, the quadratic equation has two solutions. However, only those with positive imaginary parts are acceptable as the dielectric constant, so that arg ε is constrained into the interval [0, π]. Straightforward solution of equation (2) leads to

$$\varepsilon=b\pm\left(b+\frac{\varepsilon_1\varepsilon_2}{2}\right)^{1/2}, \quad (3)$$

$$\text{with } b=\frac{(3c-1)(\varepsilon_2-\varepsilon_1)+\varepsilon_1}{4}.$$

The major disadvantage of equation (2) is that, for given values of ε1 and $\varepsilon_2$ the principal branch of the complex square root (plus sign) does not always yield the proper ε value over the whole concentration range.

The branch selection problem can be avoided by normalizing equation (1) with the respect to the refractive index of the materials mixed [2]. The dependent variable ε is first reduced to the dimensionless form

$$z=\frac{\varepsilon}{n_1n_2} \quad (4)$$

$$\text{with } n_1=\sqrt{\varepsilon_1}, n_2=\sqrt{\varepsilon_2};$$

Equation then becomes:

$$(1-c)\frac{(n_1/n_2)-z}{(n_1/n_2)+2z}=c\frac{z-(n_2/n_1)}{(n_2/n_1)+2z}, \quad (5)$$

$$\text{let } p=\frac{n_1}{n_2}. \quad (6)$$

The corresponding quadratic equation is simplified to

$$2z^2-[(3c-1)(\frac{1}{p}-p)+p]z-1=0. \quad (7)$$

The solution of the equation (7) is:

$$Z=d+(d^2+0{,}5)^{1/2}$$

with the discriminant of quadratic equation

$$d=0{,}25[(3c-1)(\frac{1}{p}-p)+p]. \quad (8)$$

According to equation (4)

$$\varepsilon=zn_1n_2. \quad (9)$$

First we compute z with equation (6) and (8), and equation (9) yields the effective dielectric constant of heterophase medium. Then using the сояелation between the real and imaginary parts of dielectric constant and refractive index и and extinction coefficient $k$ (10) we obtain the values of n and $k$

$$\varepsilon=\varepsilon'-i\varepsilon':$$

$$\varepsilon'=n^2-k^2; \quad (10)$$

$$\varepsilon''=2nk.$$

If dependence *of ξ on c* is analyzed by derivation one can notice that for any value of $c$ the arg ε is belongs to the interval [O, π]. In contrast to equation (2) the above transformed approach leads to correct values without any father sign testing for any set of n1, n2 and $c$.

## 2. Theoretical calculations and experimental results

Using Bruggman theory and experimental data of SiC and AlN refractive index and extinction coefficient, the optical properties of two-phases samples SiC + AlN type with different quantity of the aluminum nitride admixture were calculated. Reflection spectra for s- and p-polarized light were measured in the range 4000 $cm^{-1}$ (2,5 mk) to 400 $cm^{-1}$ (25 mk). The refractive index and extinction coefficient were calculated by Fresnel's formula for the next samples: SiC, AlN, SiC + 15 % AlN, SiC + 20 % AlN, SiC + 50 % AlN. The optical constants in visible and ultraviolet region ware measured by ellipsometry [3] in wavelength from 0,26 mk to 1,2mk.

The experimental and calculated spectra of refractive index and extinction coefficient in infrared are presented on fig. 1-3. The spectra in the visible and ultraviolet region are presented on fig. 4-6.

In a case when a sample consist of 15 % AlN and 85 % SiC refractive index change a little over the ultraviolet and visible region, thus there are no essential changes in crystalline structure. The reduction of extinction coefficient for this sample can connected with AlN that has less absorption in infrared. Theoretical calculation, according to Bruggman theory, gives a value of the absorption coefficient larger and a value of the extinction coefficient smaller then that obtained by the experiment.

The reason of a divergence is that Bruggman theory doesn't take into account the formation a new chemical composition on the border of phases. For samples SiC + % 20 AlN and SiC + % 50 AlN

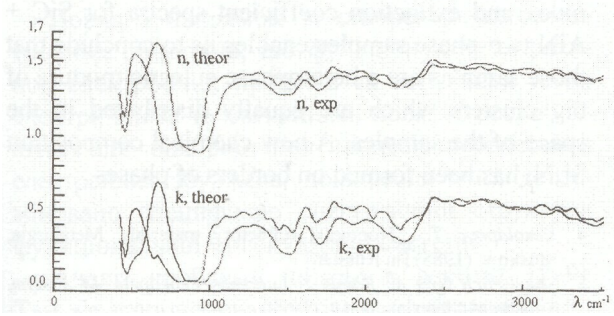


**Fig. 1. Extinction coefficient and absorption index of the sample SiC + 15 % AlN in infrared**

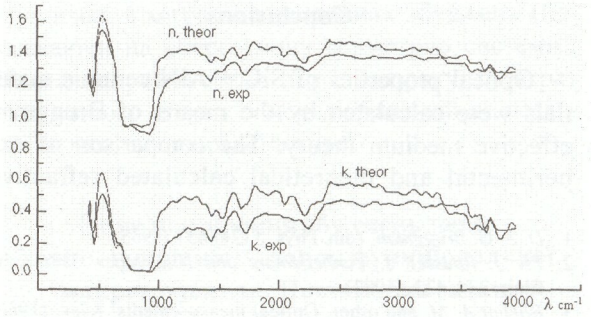


**Fig. 2. Extinction coefficient and absorption index of the sample SiC + 20 % AlN in infrared**

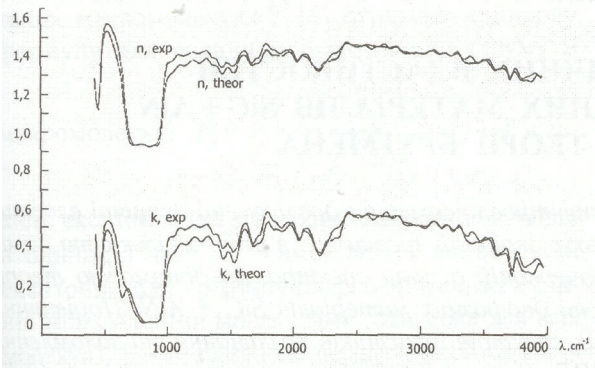


**Fig. 3. Extinction coefficient and absorption index of the sample SiC + 50 % AlN in infrared**

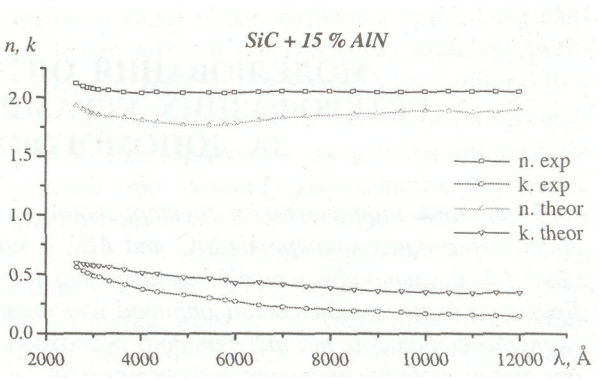


**Fig. 4. Extinction coefficient and absorption index of the sample SiC + *15 %* AlN in ultraviolet and visible wave range**

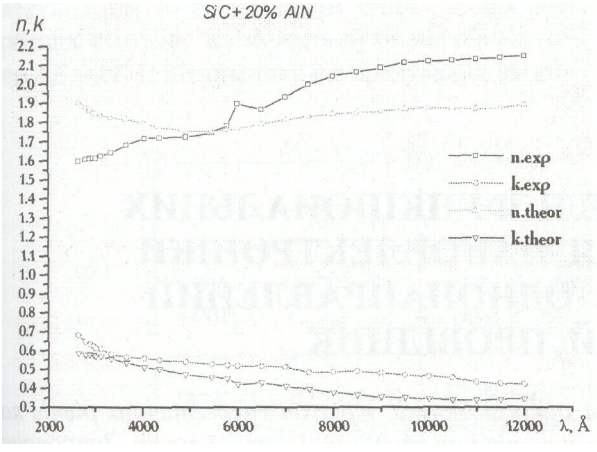


**Fig. 5. Extinction coefficient and absorption index of the sample SiC + 20 % AlN in ultraviolet and visible wave range**

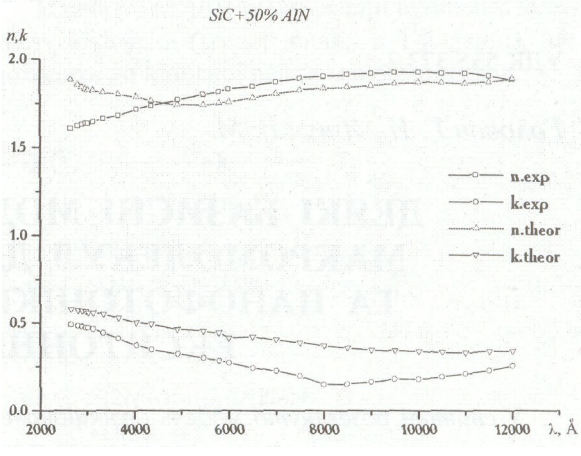


**Fig. 6. Extinction coefficient and absorption index of the sample SiC + 50 % AlN in ultraviolet and visible wave range**

one can observes the recession of refractive index, which can be explained by presence of oxygen in the AlN [4].

The experimental data of absorption coefficient increase faster then the theoretical data in the ultraviolet region. In this region $SJsN_4$ has an absorption band therefore one can conclude that a new chemical composition ($Si_3N_4$) on borders of phases in formed in the specimen manufacturing process.

The divergence between the theoretical calculated and experimental spectra is insignificant. Comparing the experimental and theoretically calculated spectra of refractive index and extinction coefficient for SiC + AlN type two-phase samples we can conclude that the SiC + AlN system is a heterophase eutectic mixture of big clusters which are equally distributed in the space of the samples [5].

## Conclusions

Optical properties of SiC + AlN ceramic materials were calculated by the means of Bruggman effective medium theory. The comparison of experimental and theoretical calculated refractive index and extinction coefficient spectra for SiC + AlN two-phase samples enables us to conclude that those samples are a heterophase eutectic mixture of big clusters which are equally distributed in the space of the samples. A new chemical composition $Si_3N_4$ has been formed on borders of phases.


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## МОДЕЛЮВАННЯ ОПТИЧНИХ ВЛАСТИВОСТЕЙ ГЕТЕРОФАЗНИХ КЕРАМІЧНИХ МАТЕРІАЛІВ SiC + AlN ЗА ДОПОМОГОЮ ТЕОРІЇ БРУҐМЕНА


*Методами інфрачервоної спектроскопії та спектроеліпсометрії досліджено оптичні властивості керамічних матеріалів SiC та AlN, а також: двофазні зразки SiC з різною кількістю домішок AlN в ультрафіолетовій, видимій та інфрачервоній ділянці спектра. За допомогою теорії Бруґмена були змодельовані оптичні властивості двофазних матеріалів SiC + AlN. Порівняння експериментальних та теоретично розрахованих спектрів показників поглинання та заломлення дає змогу зробити висновок, що система SiC + AlN- це гетерофазна евтектична механічна суміш великих кластерів, рівномірно розподілених по об'єму зразка.*