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# Effect of the defectiveness of the carbon sublattice on the elastic properties of cubic titanium carbide $TiC_y$

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Changes in the elastic constants $c_{ij}$ of disordered cubic titanium carbide $TiC_y$ with an increasing the defectiveness of the carbon sublattice are estimated for the first time. It was found that the deviation of titanium carbide from the stoichiometric composition $TiC_{1.0}$ leads to a decrease in the elastic stiffness constants $c_{ij}$ of disordered $TiC_y$ carbide with a simultaneous increase in elastic anisotropy. The distributions of Young's modulus $E$ and Poisson's ratio $\mu$ in the (100) plane and the distributions of the shear modulus $G$ in the (100), (110), and (111) planes have been calculated as functions on the crystallographic direction $[hkl]$ and on the relative carbon content $y$ in $TiC_y$ carbide. The lowest values of the shear modulus $G_{hkl}$ for $TiC_y$ are observed in the (111) plane.

**Keywords:** Titanium carbide, Nonstoichiometry, Vacancies, Elastic properties.

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## 1. Introduction

Cubic (space group $Fm\bar{3}m$) titanium carbide $TiC_y$ has the widest homogeneity range (from $\sim TiC_{0.47-0.48}$ to $TiC_{1.00}$) among all strongly nonstoichiometric carbides [1,2]. All its properties depend strongly on relative carbon content $y$ and vary significantly within the homogeneity range [1,3]. Offering high hardness and low density combined with high thermal and corrosion resistance, titanium carbide has great potential for engineering application, e.g., in tungstenless hard alloys for metal working [3,4], nanocomposites [3], hard coatings [5], and grain growth inhibitors [6].

The determination of $TiC_y$ compositions combining high mechanical characteristics with reduced brittleness and enhanced ductile properties is a crucial goal of research focused on titanium carbide. A change in the nonstoichiometry of titanium carbide may be instrumental in achieving this goal.

Data on the elastic properties of titanium carbide are needed to predict the mechanical properties of various phases of titanium carbide and determine the conditions for mechanochemical synthesis (specifically, high-energy milling) of nanocrystalline $TiC_y$ powders.

No systematic measurements of the elastic properties of disordered cubic titanium carbide $TiC_y$ as functions of its composition have been carried out to date, although certain data on bulk modulus $B$ and shear modulus $G$ of $TiC_y$ with different values of carbon content $y$ have been published [7–18].

Theoretical estimates of the elastic properties, which are normally obtained using different versions of the density functional theory with local density (LDA) and generalized gradient (GGA) approximations for exchange-correlation potentials, are available only for stoichiometric titanium carbide $TiC_{1.0}$ and were presented in [14,19–28]. The results of theoretical calculations of elastic constants $c_{ij}$ of stoichiometric $TiC_{1.0}$ carried out in different studies vary significantly: according to [14,24,25], $c_{11} \cong 470$, $c_{12} \cong 105$, and $c_{44} \cong 170$ GPa, while the authors of [20,21] provide higher estimated values of the same elastic stiffness constants (603–610, 103–124, and 173–181 GPa, respectively). Note that calculations relying on the local density approximation yield higher values of $c_{ij}$ than the calculations with GGA.

More recently, the studies into potential stable superstructures in nonstoichiometric carbides have focused on an evolutionary algorithm implemented in USPEX (Universal Structure Predictor: Evolutionary Xtallography) [29]. The elastic properties of predicted carbide superstructures are estimated by calculating the coefficients of the elasticity tensor with the use of the finite difference method [30] implemented in VASP (Vienna Ab initio Simulation Package) [31,32]. However, the software solutions mentioned above allow one to estimate only the elastic properties of ordered carbide phases (superstructures), while the elastic properties of disordered nonstoichiometric carbides remain unknown. For example, the authors of [33,34] calculated the elastic properties of the following two ordered phases of titanium carbide stable at $T = 0$ K and $P = 0$ GPa: superstructure $Ti_2C$ with trigonal and cubic symmetry and superstructure $Ti_3C_2$ with monoclinic or orthorhombic symmetry. According to [34], two tetragonal phases $Ti_2C$ and $Ti_3C_2$ are stable in titanium carbide at pressures exceeding 40 GPa.

The present study is focused on the semiempirical estimation of elastic constants $c_{ij}$ of disordered nonstoichiometric

titanium carbide $TiC_y$ as functions of its composition. The estimation is performed by analyzing simultaneously the experimental data from [7–18] on the mechanical properties of titanium carbide with different carbon content and the theoretical data on the elastic constants of stoichiometric carbide $TiC_{1.0}$. This is the first time when such an approach to estimating the elastic properties of disordered phases is applied to nonstoichiometric compounds of the family of cubic carbides of transition metals.

## 2. Results and discussion

The dependence of bulk modulus $B$ of titanium carbide $TiC_y$ on relative carbon content $y$ is plotted in Fig. 1 based on the experimental data from [7–14]. The increase in defectiveness of the carbon sublattice as a result of $y$ reduction, which decreases from 1.0 to 0.5, is accompanied by a slight ($\sim 20$ GPa) reduction in $B$. According to the approximation of the experimental $B$ values, the bulk modulus of stoichiometric carbide $TiC_{1.0}0$ is $B_{y=1} = 241.7$ GPa. Quantitatively, dependence $B(y)$ of the bulk modulus of titanium carbide on the carbon content at 300 K may be characterized in the following way:

$$B(y) = 183.5 + 98.8y - 40.6y^2$$

$$= B_{y=1}(0.75938 + 0.40879y - 0.16817y^2) \pm 10.0\,\text{GPa}. \quad (1)$$

The data from [8–10,13,15–18] on shear modulus $G$ for different compositions of carbide $TiC_y$ are presented in Fig. 2. Deviations of titanium carbide from the stoichiometric composition lead to nonlinear changes in $G$: the shear modulus first increases in the transition from $TiC_{1.0}$ to $\sim TiC_{0.92}$ and then decreases to a well-pronounced minimum in the region of $TiC_{0.87}$–$TiC_{0.81}$. As $y$ drops to $\sim 0.78$, modulus $G$ increases slightly, but then decreases monotonically as $y$ drops further to $\sim 0.55$. According to the results of the approximating calculation, the shear modulus of stoichiometric carbide $TiC_{1.00}$ is $G_{y=1} = 187.2$ GPa. Taking this result and the observed $G$ minimum into account, we may present dependence $G(y)$ of the shear modulus on carbon content $y$ of carbide $TiC_y$ at 300 K in the following form:

$$G(y) = G_{y=1}\Big[(-11.03975 + 25.74769y - 13.70794y^2) \times f_H(y - y_b) + (-0.82182 + 4.41716y - 2.76328y^2) \times f_H(y - y_b)\Big] \pm 10.0\,\text{GPa}, \quad (2)$$

where

$$f_H(y - y_b) = \begin{cases} 1, & \text{if } y \geq y_b \\ 0, & \text{if } y < y_b \end{cases}$$

is the Heaviside step function with $y_b = 0.84$.

The bulk and shear moduli of isotropic cubic crystals are related to the elastic stiffness constants in the following way: $B = (c_{11}+2c_{12})/3$ and $G = c_{44}$ [35]. We may take it as a first approximation that dependences $B(y)$ and $G(y)$ of single-crystal titanium carbide $TiC_y$ on relative carbon content $y$ have the same shape as quantitative dependences $B(y)$ (1) and $G(y)$ (2) derived from the experimental data [7–18]. In other words,

$$(c_{11} + 2c_{12})/3 \sim B_{y=1}(0.75938 + 0.40879y - 0.16817y^2)$$

and

$$c_{44} \sim G_{y=1}\big[(-11.03975 + 25.74769y - 13.70794y^2) \times f_H(y - y_b) + (-0.82182 + 4.41716y - 2.76328y^2) \times f_H(y - y_b)\big].$$

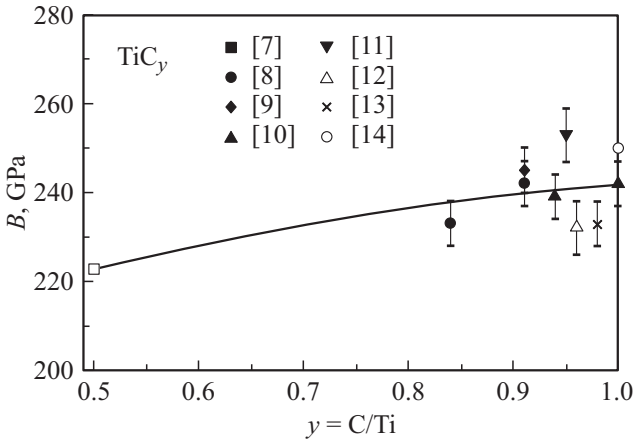


**Figure 1.** Variation of bulk modulus $B$ in the region of homogeneity of disordered cubic titanium carbide $TiC_y$ at 300 K: ■ — [7], ● — [8], ◆ — [9], ▲ — [10], ▼ — [11], △ — [12], × — [13], ○ — [14]. Approximating dependence $B(y)$ is represented by the solid curve.

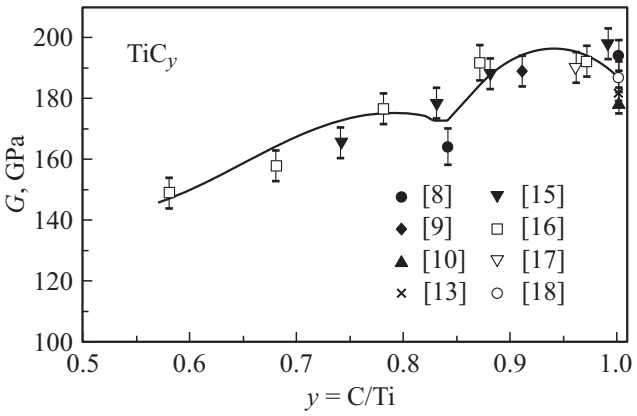


**Figure 2.** Dependence of shear modulus $G$ on the composition of disordered cubic titanium carbide $TiC_y$ at a temperature of 300 K: ● — [8], ◆ — [9], ▲ — [10], × — [13], ▼ — [15], □ — [16], △ — [17], ○ — [18]. Approximating dependence $G(y)$ is represented by the solid curve.

Elastic stiffness constants $c_{ij}$ (GPa), elastic compliance constants $s_{ij}$ ($Pa^{-1}$), and elastic anisotropy criterion $A_{an}$ for titanium carbide $TiC_y$ with varying carbon content $y$

| $y$ | $c_{11}$ | $c_{12}$ | $c_{44}$ | $s_{11}$ | $s_{12}$ | $s_{44}$ | $A_{an}$ |
|---|---|---|---|---|---|---|---|
| 0.50 | 478.4 | 106.0 | 127.4 | $2.273 \cdot 10^{-12}$ | $-0.412 \cdot 10^{-12}$ | $7.852 \cdot 10^{-12}$ | 0.684 |
| 0.55 | 484.4 | 107.3 | 141.2 | $2.245 \cdot 10^{-12}$ | $-0.407 \cdot 10^{-12}$ | $7.081 \cdot 10^{-12}$ | 0.749 |
| 0.60 | 490.0 | 108.6 | 152.6 | $2.219 \cdot 10^{-12}$ | $-0.403 \cdot 10^{-12}$ | $6.555 \cdot 10^{-12}$ | 0.800 |
| 0.65 | 495.1 | 109.7 | 161.4 | $2.196 \cdot 10^{-12}$ | $-0.398 \cdot 10^{-12}$ | $6.197 \cdot 10^{-12}$ | 0.837 |
| 0.70 | 499.9 | 110.8 | 167.7 | $2.175 \cdot 10^{-12}$ | $-0.395 \cdot 10^{-12}$ | $5.964 \cdot 10^{-12}$ | 0.862 |
| 0.75 | 504.1 | 111.7 | 171.4 | $2.157 \cdot 10^{-12}$ | $-0.391 \cdot 10^{-12}$ | $5.834 \cdot 10^{-12}$ | 0.874 |
| 0.80 | 508.0 | 112.6 | 172.6 | $2.141 \cdot 10^{-12}$ | $-0.388 \cdot 10^{-12}$ | $5.792 \cdot 10^{-12}$ | 0.873 |
| 0.85 | 511.4 | 113.3 | 172.3 | $2.126 \cdot 10^{-12}$ | $-0.386 \cdot 10^{-12}$ | $5.802 \cdot 10^{-12}$ | 0.866 |
| 0.90 | 514.4 | 114.0 | 188.4 | $2.114 \cdot 10^{-12}$ | $-0.383 \cdot 10^{-12}$ | $5.307 \cdot 10^{-12}$ | 0.941 |
| 0.95 | 516.9 | 114.5 | 192.0 | $2.104 \cdot 10^{-12}$ | $-0.382 \cdot 10^{-12}$ | $5.209 \cdot 10^{-12}$ | 0.954 |
| 1.00 | 519.0 | 115.0 | 183.0 | $2.095 \cdot 10^{-12}$ | $-0.380 \cdot 10^{-12}$ | $5.465 \cdot 10^{-12}$ | 0.906 |

According to [36], dependences $c_{11}(y)$ and $c_{12}(y)$ of the elastic constants on the composition of cubic carbides are identical. The theoretical values of $B_{\mathrm{calc},y=1} = 249$ and $G_{\mathrm{calc},y=1} = 190$ GPa moduli of stoichiometric titanium carbide calculated within GGA in [22] and $B_{\mathrm{calc},y=1} = 250$ GPa are the closest to the experimental values of $B_{y=1} = 241.7$ and $G_{y=1} = 187.2$ GPa. Taking this and the introduced approximation into account, we may present dependences $c_{ij}(y)$ of the elastic constants on the composition of carbide $TiC_y$ in the following form:

$$c_{11}(y) = c_{11}(y=1)[0.75938 + 0.40879y - 0.16817y^2], \tag{3a}$$

$$c_{12}(y) = c_{12}(y=1)[0.75938 + 0.40879y - 0.16817y^2], \tag{3b}$$

$$c_{44}(y) = c_{44}(y=1)[(-11.03975 + 25.74769y - 13.70794y^2) f_{\mathrm{H}}(y - y_b) + (-0.82182 + 4.41716y - 2.76328y^2) f_{\mathrm{H}}(y - y_b)], \tag{3c}$$

$$f_{\mathrm{H}}(y - y_b) = \begin{cases} 1, & \text{if } y \geq y_b \\ 0, & \text{if } y < y_b \end{cases}$$

is the Heaviside step function with $y_b = 0.84$; $c_{11}(y=1) = 519$ GPa, $c_{12}(y=1) = 115$ GPa, and $c_{44}(y=1) = 183$ GPa [22].

Elastic stiffness constants $c_{11}, c_{12}, c_{44}$ and elastic compliance constants $s_{11}, s_{12}, s_{44}$ for cubic crystals are related in the following way: $s_{44} = 1/c_{44}$, $s_{11} = (c_{11} + c_{12})/[(c_{11} - c_{12})(c_{11} + 2c_{12})]$ and $s_{12} = = -c_{12}/[(c_{11} - c_{12})(c_{11} + 2c_{12})]$ [35].

The estimates of elastic stiffness constants $c_{ij}$ and components $s_{ij}$ of the compliance tensor of titanium carbide $TiC_y$ are presented in the table.

Young's modulus $E_{hkl}$ and Poisson's ratio $\mu_{hkl}$ of cubic crystals are anisotropic and depend on crystallographic direction $[hkl]$. These elastic characteristics are expressed in terms of components $s_{11}$, $s_{12}$, and $s_{44}$ of the compliance tensor as [37]

$$E_{hkl} = \frac{1}{s_{11} - 2(s_{11} - s_{12} - \frac{1}{2}s_{44})\Gamma}, \tag{4}$$

$$\mu_{hkl} = -\frac{s_{12} + (s_{11} - s_{12} - \frac{1}{2}s_{44})\Gamma}{s_{11} - 2(s_{11} - s_{12} - \frac{1}{2}s_{44})\Gamma}, \tag{5}$$

where

$$\Gamma = \frac{h^2k^2 + h^2l^2 + k^2l^2}{(h^2 + k^2 + l^2)^2}$$

is the anisotropy factor of cubic crystals.

Taking Eqs. (4) and (5) into account, we derive the following expressions for shear $G_{hkl}$ and bulk $B$ moduli:

$$G_{hkl} = \frac{1}{2s_{11} - 2s_{12} - 6(s_{112} - s_{12} - s_{44}/2)\Gamma}, \tag{6}$$

$$B = 1/[3(s_{11} + 2s_{12})]. \tag{7}$$

It follows from Eq. (7) that bulk modulus $B$ of cubic crystals does not depend on direction $[hkl]$ and is isotropic.

The availability of data on elastic constants $c_{11}, c_{12}, c_{44}$, and $s_{11}, s_{12}, s_{44}$ of carbide $TiC_y$ with different degrees of defectiveness of the carbon sublattice (see the table) provided an opportunity to determine the distributions of elastic properties of single-crystal cubic carbide $TiC_y$ as functions of direction $[hkl]$ and relative carbon content $y$. Fig. 3 shows the calculated distributions of Young's modulus $E$, shear modulus $G$, and Poisson's ratio $\mu$ of cubic carbide $TiC_y$. The distributions of Young's modulus $E_{hkl}$ in plane (100) are presented for carbides $TiC_y$ with $y = 0.5$, 0.6, 0.7, 0.8, and 1.0 (see Fig. 3). The distributions of Young's modulus $E_{hkl}$ in planes (010) and (001) have the same shape. Young's modulus $E_{hk0}$ of carbide $TiC_{1.0}$ in plane (100) varies from $\sim 449.7$ to $\sim 477.3$ GPa, while the Young's modulus of nonstoichiometric carbide $TiC_{0.5}$ with a defect carbon sublattice containing 50% of vacancies varies from $\sim 345.7$ to $\sim 439.9$ GPa in the same plane. The maximum value of shear modulus $G_{hk0}$ increases slightly from $\sim 186.2$

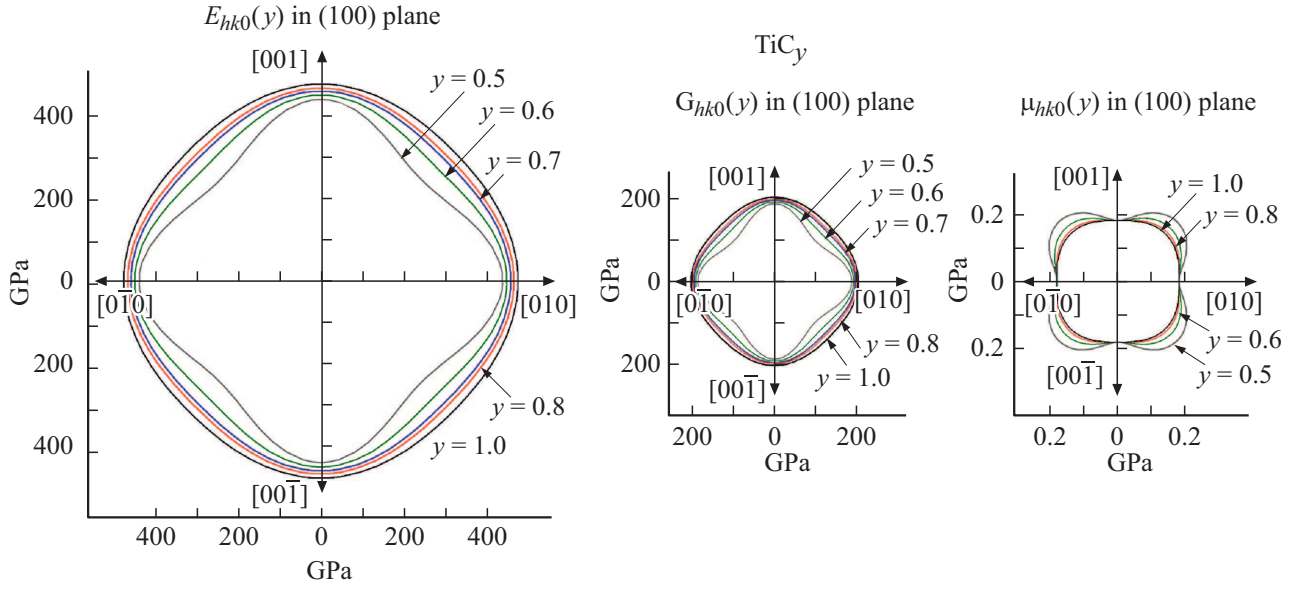


**Figure 3.** Dependences of Young's modulus $E$, shear modulus $G$, and Poisson's ratio $\mu$ on crystallographic direction $[hkl]$ in plane (100) of cubic carbide TiC$_y$ with relative carbon content $y$ varying from 0.5 to 1.0.

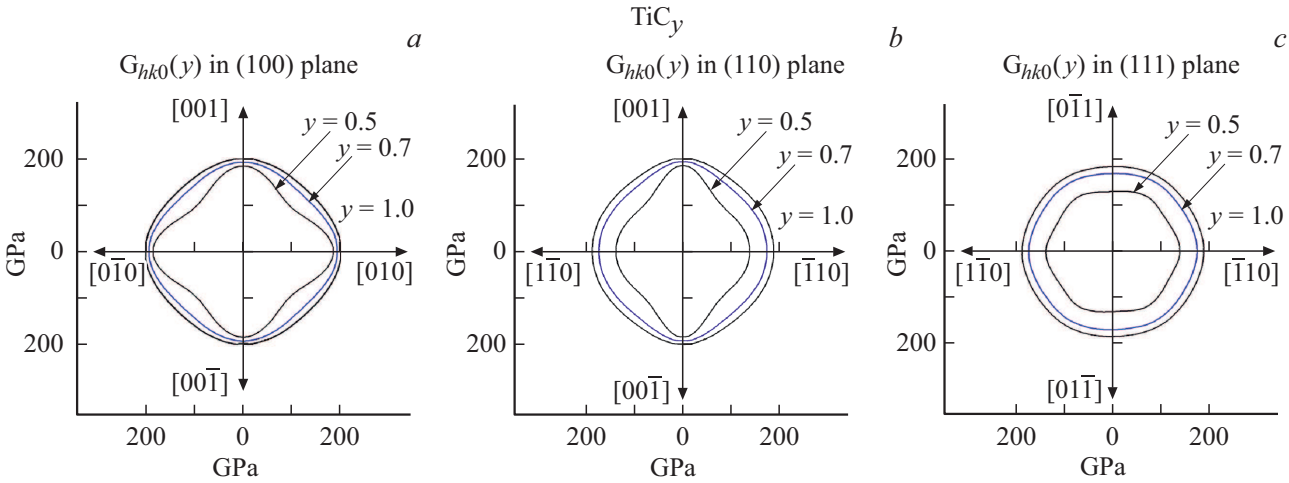


**Figure 4.** Distributions of shear modulus $G_{hkl}$ with crystallographic direction $[hkl]$ in planes (*a*) (100), (*b*) (110), and (*c*) (111) of cubic carbide TiC$_y$ with different carbon content $y$.

to $\sim 202.0$ GPa in the transition from nonstoichiometric carbide TiC$_{0.5}$| to stoichiometric TiC$_{1.0}$. The increased defectiveness of the carbon sublattice of titanium carbide translates into an increased Poisson's ratio $\mu$: in plane (100), the maximum value of $\mu$ of stoichiometric and nonstoichiometric carbides TiC$_{1.0}$ and TiC$_{0.5}$ is $\sim 0.200$ and $\cong 0.250$, respectively (see Fig. 3). Bulk modulus $B$ of cubic titanium carbide TiC$_y$ is isotropic and depends only on carbon content $y$: the value of $B$ varies from $\sim 230.1$ GPa for TiC$_{0.5}$ to $\sim 249.7$ GPa for stoichiometric TiC$_{1.0}$.

Fig. 4 shows the calculated dependences of shear modulus $G_{hkl}$ of carbide TiC$_y$ on crystallographic direction $[hkl]$. The distributions of shear modulus $G$ in planes (100), (110), and (111) are presented for carbides TiC$_y$ with $y = 0.5$, 0.7, and 1.0. The lowest $G_{hkl}$ value for carbides TiC$_y$ is found in plane (111). Shear modulus $G_{hkl}$ in plane (111) is almost direction-independent and varies only slightly from $\sim 184$ to $\sim 187$ GPa for TiC$_{1.0}$ and from $\sim 130$ to $\sim 138$ GPa for TiC$_{0.5}$ (Fig. 4, *c*).

Simple criterion $A_{an} = 2c_{44}/(c_{11} - c_{12})$ was proposed in [38] as a variable to be used to characterize quantitatively the anisotropy of elastic properties of cubic crystals. The value of $A_{an}$ for isotropic cubic crystals is 1. According to [38], the anisotropy of elastic properties grows stronger as the value of $A_{an}$ deviates further from 1. The calculated values of $A_{an}$ (see the table) demonstrate that the variation of the composition of titanium carbide from a near-stoichiometric composition TiC$_{1.0-0.95}$ to carbide TiC$_{0.50}$ with the highest defectiveness of the carbon sublattice coincides with a reduction in $A_{an}$, which drops from

$\sim 0.91-0.95$ to $\sim 0.68$. Thus, the anisotropy of the elastic properties of disordered titanium carbide grows stronger as the defectiveness of its carbon sublattice increases.

Using the obtained data on elastic constants $c_{ij}$ and $s_{ij}$ of disordered cubic titanium carbide $TiC_y$ with different relative carbon content $y$, one may determine the Debye temperatures and the lattice (phonon) heat capacities of various compositions of carbide $TiC_y$.

According to the Voigt–Reuss–Hill averaging method [39], bulk moduli $B$ and shear moduli $G$ are related to the elastic constants in the following way:

$$B_{\mathrm{V}} = \left[c_{11} + c_{22} + c_{33} + 2(c_{12} + c_{13} + c_{23})\right]/9, \quad (8a)$$

$$B_{\mathrm{R}} = 1/\left[s_{11} + s_{22} + s_{33} + 2(s_{12} + s_{13} + s_{23})\right], \quad (8b)$$

$$G_{\mathrm{V}} = \left[c_{11} + c_{22} + c_{33} + 3(c_{44} + c_{55} + c_{66}) - (c_{12} + c_{13} + c_{23})\right]/15, \quad (8c)$$

$$G_{\mathrm{R}} = 15/\left[4(s_{11} + s_{22} + s_{33}) - 4(s_{12} + s_{13} + s_{23}) + 3(s_{44} + s_{55} + s_{66})\right], \quad (8d)$$

while the average values of isotropic moduli are defined as follows:

$$B = (B_{\mathrm{V}} + B_{\mathrm{R}})/2, \quad G = (G_{\mathrm{V}} + G_{\mathrm{R}})/2. \quad (9)$$

If density $\rho$ is known, one may calculate longitudinal $v_L$, transverse $v_t$, and mean $v_m$ velocities of propagation of elastic oscillations (sound velocities) [40,41] using isotropic moduli $B$ and $G$ or carbide $TiC_y$:

$$v_{\mathrm{L}} = \sqrt{(3B + 4G)/3\rho}, \quad v_t = \sqrt{G/\rho},$$

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_{\mathrm{L}}^3}\right)\right]^{-1/3}. \quad (10)$$

Having determined mean velocity $v_m$ of propagation of elastic oscillations, one may estimate the Debye temperature [41]:

$$\theta_{\mathrm{D}} = \frac{h}{k_{\mathrm{B}}}\left(\frac{3nN_A\rho}{4\pi M}\right)^{1/3} v_m\,[\mathrm{K}]. \quad (11)$$

The obtained Debye temperature value provides an opportunity to calculate the heat capacity of any carbide $TiC_y$. With the contribution of optical vibrations neglected, the lattice Debye contribution to the heat capacity of carbide $TiC_y$ takes the form

$$C_{\mathrm{D}} = (1 + y)\,\frac{12\pi^4 k_{\mathrm{B}} N_A}{5}\left(\frac{T}{\theta_{\mathrm{D}}}\right)^3. \quad (12)$$

Literature data on the heat capacity of $TiC_y$ are limited to its estimate obtained in [42] based on the results of neutron diffraction measurements. It would be instructive if the authors of [42] continued their research by estimating the heat capacity of $TiC_y$ based on the presented data on the elastic constants.

## 3. Conclusion

In essence, this study is the first to determine elastic constants $c_{ij}$ and $s_{ij}$ as functions of carbon content $y$ in the region of homogeneity ($TiC_{0.5}-TiC_{1.0}$) of nonstoichiometric disordered cubic titanium carbide $TiC_y$. The analysis undertaken revealed that elastic stiffness constants $c_{ij}$ of disordered carbide $TiC_y$ decrease as the defectiveness of the carbon sublattice of titanium carbide increases. The increase in defectiveness of the carbon sublattice of carbide $TiC_y$ is accompanied by an increase in anisotropy of its elastic properties.

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### Conflict of interest

The author declares that he has no conflict of interest.

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