



## ANISOTROPIC BEHAVIOUR OF ULTRASONIC WAVE PROPAGATION IN TiC AND TiN SINGLE CRYSTALS AT HIGH TEMPERATURES

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# ANISOTROPIC BEHAVIOUR OF ULTRASONIC WAVE PROPAGATION IN TiC AND TiN SINGLE CRYSTALS AT HIGH TEMPERATURES

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## ABSTRACT

Understanding the anisotropic behavior of materials is fundamental for optimizing their performance in various industrial and technological applications. This study investigates the anisotropic nature of ultrasonic wave propagation through titanium carbide (TiC) and titanium nitride (TiN) crystals, two materials of significant interest due to their mechanical and electrical properties. Utilizing theoretical approach starting from nearest neighbor distance and hardness parameter, we systematically characterize the elastic properties and acoustic wave propagation behavior for these crystals using Coulomb and Born-Mayer potentials. By computing ultrasonic wave velocity along different crystallographic directions, we unveil substantial directional dependencies in wave velocity indicative of pronounced anisotropy in both TiC and TiN. Our findings reveal significant directional dependencies in the velocity of ultrasonic waves, indicating pronounced anisotropy in both materials. Through careful analysis, we elucidate the underlying mechanisms contributing to this anisotropic behavior, which stem from the crystal lattice structure and bonding configurations. Beyond fundamental insights, our study underscores the practical implications of these anisotropic characteristics in engineering applications. TiC and TiN have fcc crystal structure and find use in diverse fields such as harden and protect the cutting and sliding surfaces and also in heat shield coating. The directional variations in ultrasonic wave propagation observed in this study have direct implications for optimizing the performance of such applications. This study not only advances the understanding of anisotropic materials behavior but also provides actionable insights for harnessing the unique properties of TiC and TiN crystals in engineering applications.

**Keywords:** Titanium Carbide, Crystallographic Directions, Wave Velocity, Configurations, Materials Behavior, Properties

## INTRODUCTION

The directional dependence of material properties plays an important role in shaping the performance and functionality of various materials in diverse technological applications. Understanding the anisotropic behaviour of materials is crucial for optimizing their properties and designing efficient systems tailored to specific needs. In this context, the investigation of ultrasonic wave propagation through materials offers valuable insights into their elastic properties and structural characteristics.

The scientific community has shown great interest in transition metal carbides and nitrides, owing to their high melting points, exceptional hardness, and distinctive combination of electrical and thermal conductivities. Titanium carbide (TiC) and titanium nitride (TiN) are two materials that have garnered significant attention owing to their exceptional mechanical and electrical properties. These materials, with their face-centered cubic (fcc) crystal structure,

find widespread use in applications requiring hardness, wear resistance, and thermal stability, such as coatings for cutting tools, sliding surfaces, and heat shields. These crystals exhibit unusual physical and mechanical characteristics and show rock salt structure forming covalent bonding, which is typical for ionic crystals [1, 2]. The study of the second-order elastic constants (SOECs) and ultrasonic wave velocities along different anisotropic axes are also equally important to discuss the various fundamental solid-state phenomena which include inter-atomic potentials, equation of state, phonon spectra etc. [3, 4]. If the values of SOECs and lattice density at a particular temperature are known, the ultrasonic velocities for longitudinal and shear waves can be computed, which give an important information about its anisotropic properties.

In a deformed crystal, the elastic energy density can be expressed as a strain-dependent power series

derived from Taylor expansion. The coefficients corresponding to the second-, third-, and fourth-order terms in this series are referred to as second-order, third-order, and fourth-order elastic constants (SOECs, TOECs, and FOECs), respectively. The present paper is mainly focussed on the study of temperature variation of second order elastic constants and ultrasonic wave velocities along different anisotropic axes for TiC and TiN crystals from 300-1000 K using Born-Mayer and Coulomb potential starting from the nearest neighbour distance and hardness parameter. These crystals are well known due to their potential applications. These are frequently used in coating materials for surface protection of cutting tools, electrically conducting barrier, aerospace structural components, thin films for efficient electronic devices and applying highly corrosion-resistant coatings to enhance the surface protection of cutting tools [5-10]. The identified anisotropic behaviour has direct implications for optimizing the performance of coatings, cutting tools, and other applications where mechanical and thermal stability are paramount.

### THEORY

For crystals exhibiting cubic symmetry, the elastic energy density may be represented as a strain-dependent expansion up to fourth-order terms [11].

$$U_0 = U_2 + U_3 + U_4$$

$$= [1/2!] C_{ijkl} \alpha_{ij} \alpha_{kl} + [1/3!] C_{ijklmn} \alpha_{ij} \alpha_{kl} \alpha_{mn} + [1/4!] C_{ijklmnpq} \alpha_{ij} \alpha_{kl} \alpha_{mn} \alpha_{pq} \quad \dots(1)$$

where  $C_{ijkl}$ ,  $C_{ijklmn}$  and  $C_{ijklmnpq}$  are the SOECs, TOECs and FOECs in tensorial form;  $\alpha_{ij}$  are the Lagrangian strain components. The SOECs, TOECs and FOECs are as given below:

$$C_{ijkl} = C_{IJ} = \left( \frac{\partial^2 U}{\partial \alpha_{ij} \partial \alpha_{kl}} \right)_{\alpha=0}$$

$$C_{ijklmn} = C_{IJK} = \left( \frac{\partial^3 U}{\partial \alpha_{ij} \partial \alpha_{kl} \partial \alpha_{mn}} \right)_{\alpha=0}$$

$$\text{and } C_{ijklmnpq} = C_{IJKL} = \left( \frac{\partial^4 U}{\partial \alpha_{ij} \partial \alpha_{kl} \partial \alpha_{mn} \partial \alpha_{pq}} \right)_{\alpha=0} \quad \dots(2)$$

where  $C_{IJ}$ ,  $C_{IJK}$  and  $C_{IJKL}$  are the SOECs, TOECs and FOECs in Brügger's definition and Voigt notations [12]. The free energy density of a crystal at a finite temperature T is

$$U_{Total} = U_0 + U^{vib}$$

An elastic constant consists of two parts as follows:

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{vib}, \quad C_{IJK} = C_{IJK}^0 + C_{IJK}^{vib} \quad \text{and}$$

$$C_{IJKL} = C_{IJKL}^0 + C_{IJKL}^{vib} \quad \dots(3)$$

The ultrasonic velocities can be computed using the values of  $C_{ij}$ 's and density  $\rho$  with the help of following expressions for velocities.

Along the <100> crystallographic direction

$$V_l = \sqrt{\frac{C_{11}}{\rho}}$$

$$V_s = \sqrt{\frac{C_{44}}{\rho}} \quad \dots(4)$$

Along the <110> crystallographic direction

$$V_l = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\rho}}$$

$$V_{s1} = \sqrt{\frac{C_{44}}{\rho}}$$

$$V_{s2} = \sqrt{\frac{C_{11} - C_{12}}{\rho}} \quad \dots(5)$$

Along the <111> crystallographic direction

$$V_l = \sqrt{\frac{C_{11} + 2C_{12} + 4C_{44}}{3\rho}}$$

$$V_{s1} = V_{s2} = \sqrt{\frac{C_{11} - C_{12} + C_{44}}{3\rho}} \quad \dots(6)$$

where  $V_l$  and  $V_s$  refers to longitudinal and shear wave velocities.

### RESULTS

The second order elastic constants from 300 -1000 K are given in Table 1. For both the crystals the increasing value of  $C_{11}$  with temperature shows that increased atomic motion contribute to enhanced stiffness along certain crystallographic directions, leading to an increase in  $C_{11}$  with temperature. A decrease in the value of  $C_{12}$  with an increase in temperature suggests a weakening of the material's resistance to shear deformation. An increase in the elastic constant  $C_{44}$  with an increase in temperature suggests a strengthening of the material's resistance to shear deformation in the direction associated with  $C_{44}$ .

The ultrasonic wave velocities along different crystallographic directions are given in Tables 2-4. The data show that for all the directions <100>, <110> and <111> an increase in longitudinal wave and shear wave velocity with temperature.

**TABLE 1.** SOECs in  $10^{10}$  N/m<sup>2</sup> in the Temperature range 300-1000 K.

Temp(K)	$C_{11}$		$C_{12}$		$C_{44}$	
	TiC	TiN	TiC	TiN	TiC	TiN
300	28.30807	28.55189	19.05389	20.69616	19.38779	21.03479
400	28.44743	28.69896	18.96517	20.60612	19.40181	21.05019
500	28.61560	28.87366	18.87515	20.51518	19.41767	21.06745
600	28.80061	29.06430	18.78504	20.4243	19.43457	21.08574
700	28.99607	29.26477	18.69509	20.33363	19.45211	21.10465
800	29.19839	29.47165	18.60533	20.24317	19.47005	21.12397
900	29.40543	29.68295	18.51573	20.15289	19.48828	21.14356
1000	29.61584	29.89738	18.42626	20.06275	19.50670	21.16335

**TABLE 2** Ultrasonic wave velocities along  $\langle 100 \rangle$  in  $10^3$  m/sec in the Temperature range 300-1000 K.

Temp(K)	$V_l$		$V_s$	
	TiC	TiN	TiC	TiN
300	2.39382	2.29307	1.98107	1.96820
400	2.39970	2.29896	1.98179	1.96892
500	2.40678	2.30595	1.98260	1.96972
600	2.41455	2.31355	1.98346	1.97058
700	2.42273	2.32152	1.98435	1.97146
800	2.43117	2.32971	1.98527	1.97236
900	2.43977	2.33804	1.98620	1.97328
1000	2.44849	2.34647	1.98714	1.97420

**TABLE 3** Ultrasonic wave velocities along  $\langle 110 \rangle$  in  $10^3$  m/sec in the Temperature range 300-1000 K.

Temp(K)	$V_l$		$V_{s1}$		$V_{s2}$	
	TiC	TiN	TiC	TiN	TiC	TiN
300	2.95268	2.89976	1.98107	1.96820	1.36869	1.20280
400	2.95403	2.90115	1.98179	1.96892	1.38545	1.22081
500	2.95591	2.90303	1.98260	1.96972	1.40419	1.24069
600	2.95812	2.90519	1.98346	1.97058	1.42388	1.26141
700	2.96052	2.90753	1.98435	1.97146	1.44402	1.28248
800	2.96306	2.90998	1.98527	1.97236	1.46435	1.30366
900	2.96569	2.91252	1.98620	1.97328	1.48472	1.32479
1000	2.96838	2.91511	1.98714	1.97420	1.50502	1.34579

**TABLE 4** Ultrasonic wave velocities along  $\langle 111 \rangle$  in  $10^3$  m/sec in the Temperature range 300-1000 K.

Temp(K)	$V_l$		$V_{s1} = V_{s2}$	
	TiC	TiN	TiC	TiN
300	3.11678	3.07551	1.39020	1.33173
400	3.11698	3.07579	1.39606	1.33754
500	3.11754	3.07641	1.40267	1.34401
600	3.11832	3.07723	1.40967	1.35084
700	3.11925	3.07817	1.41690	1.35787
800	3.12027	3.07920	1.42427	1.36501
900	3.12136	3.08029	1.43171	1.37221
1000	3.12250	3.08142	1.43919	1.37945

## CONCLUSIONS

1. The comparable variation in SOECs across both crystals indicates a similarity in their elastic behavior and the strengthening of the material's resistance to shear deformation makes the material suitable for the purpose where coating is required to use the material under high temperature conditions.
2. The reason for an increase in ultrasonic wave velocity with temperature is thermal stiffening. At elevated temperatures, the increased thermal energy causes atoms to vibrate more vigorously. In these materials, this can result in a stiffer response to ultrasonic waves, leading to an increase in wave velocity. These properties make the material suitable for aerospace and high temperature applications.
3. As velocities increase at nearly the same rate with temperature, which shows the similar elastic behaviour in both TiC and TiN. Both materials show excellent stability, reinforcing their use in

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high-temperature environments like cutting tools, coatings, and aerospace components.

4. The increase in wave velocity could also be related to changes in the phonon dispersion relations with temperature. This type of behaviour is verified by various investigators also [13-15].
5. The findings and their sequence presented in this study align well with those reported by other researchers [16-21] for divalent face-centered cubic (fcc) solids, thereby supporting the validity of the current theoretical framework for evaluating anharmonic properties.

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