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Theoretical Approach to Investigate Temperature Dependent Ultrasonic and Thermophysical Properties of Ti-Zr-Hf Ternary Alloy

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Abstract: ***In this study, we have computed temperature dependent ultrasonic and thermophysical properties of hcp medium entropy alloy Ti-Zr-Hf in temperature range of 0K-900K. Second order and third order elastic constants (SOECs and TOECs) have been calculated using lattice parameters using the Lennard-Jones potential model. With the help of SOECs and TOECs, the elastic parameters such as bulk modulus, shear modulus, Young's modulus, Poisson's ratio have been computed. SOECs were also utilized to determine the ultrasonic velocities at different angle along unique axis. Further, thermophysical properties such as Debye temperature, Debye heat capacity, energy density in temperature range of 0K-900K and thermal conductivity in temperature range of 300K-900K have also been theoretically estimated. Additionally, the ultrasonic attenuation due to phonon-phonon interaction in both longitudinal and shear mode and thermoelastic mechanism have been computed for chosen alloy in the temperature range 300K-900K and attenuation due to the phonon-phonon interaction was found to be dominating over that due to thermoelastic mechanism.***

Keywords: thermo-elastic properties, ultrasonic behaviour, refractory high-entropy alloys, rare-earth, hexagonal closed-packed

I. INTRODUCTION

In recent decades, refractory high entropy alloys (RHEAs) have gained a lot of attention from researchers due to their excellent thermophysical properties and widespread applications[1]–[3]. High entropy alloys (HEAs) are defined as solid solution of five or more metal elements in single phase[4]. These alloys are considered to be stabilized by high configurational entropy of mixing[5]. Alloys consisting of three or four elements are known as medium entropy alloys (MEAs). HEAs demonstrate many remarkable properties such as high tensile strength[6], ductility[7], excellent resistance to wear, corrosion, fatigue and oxidation and these properties make them promising class of materials for applications in extreme environments such as cryogenics[8], [9]. Refractory elements such as Ti, Zr, Hf, Nb etc. are known for their excellent resistant to heat, wear and to high temperature oxidation[10] and these properties make them good elements for HEAs. In literature, most of the studies of RHEAs have been based on face-centred-cubic (FCC) or body-centred-cubic (BCC)[6], [7], [11]–[13] with a very few on hexagonal closed-packed (HCP) structures[5], [14]–[16].

Elastic properties provide fundamental insight into crystal structure and nature of bonding in materials, and help in predicting the mechanical behaviour of materials. Thermophysical properties such as Debye temperature, Debye heat capacity, thermal conductivity help estimate how they behave at different temperature.

Considering these remarkable properties of RHEAs, HCP Ti-Zr-Hf becomes a promising alloy for high pressure and temperature industrial applications. Duan et al.[5] have studied the second order elastic constants (SOECs), elastic moduli at room temperature of HCP ternary alloy Ti-Zr-Hf using first principles method. Huang et al.[17] have investigated HCP ternary and quaternary alloys of Sc-Ti-Zr-Hf for their thermoelastic properties including SOECs, elastic moduli and coefficients of thermal expansion (CTE) at different temperatures.

In spite of these studies, temperature dependence of third order elastic constants (TOECs), thermophysical properties such as Debye temperature, heat capacity, thermal conductivity and ultrasonic behaviour of the Ti-Zr-Hf HCP alloy are yet to be studied. This motivates us to investigate these properties.

This study presents the theoretical investigation of temperature dependent SOECs, TOECs, ultrasonic velocities along different direction in the crystal, Debye average velocity, Debye temperature, heat capacity, energy density, thermal conductivity and ultrasonic attenuation for Ti-Zr-Hf HCP alloy.

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II. THEORY

The temperature dependence of SOECS and TOECs for Ti-Zr-Hf alloy have been evaluated using Lennard-Jones potential method. The formulation for calculation of six independent SOECs and ten independent TOECs is thoroughly discussed in the literature[18]–[21]. The bulk modulus (B), shear modulus (G), Young's modulus (Y) and Poisson's ratio have been computed by Voigt-Reuss-Hill method[22] for hexagonal crystals. The ultrasonic velocities in longitudinal (V_L), quasi-shear (V_{S1}) and shear (V_{S2}) modes along unique axis (c-axis) at different angles of propagation, Debye average velocity (V_D) and Debye temperature (θ_D) can be calculated with the help of higher order elastic constants using the formulation discussed in literature[16], [18], [20], [21].

The RHEAs are used in harsh conditions including high pressure and temperature, so it becomes important to study thermophysical properties such as heat capacity, energy density and thermal conductivity at different temperatures. The heat capacity (C_V) and thermal energy density (E_0) is evaluated using the Debye model for heat capacity[18], [23], [24].

The lattice thermal conductivity κ has been evaluated using the formulation developed by Morelli and Slack[25]:

$$\kappa = A\frac{M_a{\theta_D}^3\delta}{\gamma^2 T n^{\frac{2}{3}}} \#(1)$$

Where A is a proportionality constant (with very slightly dependence on γ), δ (in Å) is the cube root of volume per atom, n is the number of atoms per unit cell, M_a (in amu) is average atomic mass, T is the temperature (in K), γ is Grüneisen constant which can be calculated by $\gamma = \frac{\alpha B}{C_V \rho}$ where α is the volume thermal expansion coefficient, B is bulk modulus, C_V is heat capacity and ρ is density of the material.

The ultrasonic attenuation in solids and liquids is directly related to the physical properties like elasticity, thermal conductivity, type of bonds and interactions in the material etc. The lead causes for the ultrasonic attenuation in materials at high temperature are phonon-phonon interaction (Akhiezer loss)[21], [26] and loss due to thermo-elastic relaxation mechanism[16], [27]. The formulation for evaluating the ultrasonic absorption coefficient (α) over frequency (f) squared $\left(\alpha/f^2\right)$ due to phonon-phonon interaction for longitudinal and shear modes in terms of the acoustic coupling constant (D) was developed by Mason and Bateman[28] and is given as follows:

$$\left(\alpha/f^2\right) = \frac{4\pi^2 \tau_{th} E_0 D}{2\rho V^3} \#(2)$$

$$D = 9\langle\left(\gamma_i^j\right)^2\rangle - \frac{3\langle\gamma_i^j\rangle^2 C_V T}{E_0} \#(3)$$

Where V is ultrasonic velocity in longitudinal and shear modes, $\langle\left(\gamma_i^j\right)^2\rangle$ and $\langle\gamma_i^j\rangle^2$ are square average and average square Grüneisen parameters, respectively for longitudinal and shear modes and $\tau_{th} = \frac{3\kappa}{C_V V_D^2}$ is thermal relaxation time.

The ultrasonic loss due to thermoelastic relaxation mechanism is calculated by:

$$\left(\frac{\alpha}{f^2}\right)_{th} = \frac{4\pi^2\langle\gamma_i^j\rangle^2 \kappa T}{2\rho V_L^5} \#(4)$$

III.RESULT AND DISCUSSION

The SOECs and TOECs in the temperature range of 0K-900K have been computed using lattice parameters available in the literature[17] and presented in Fig. 1 and Fig. 2.

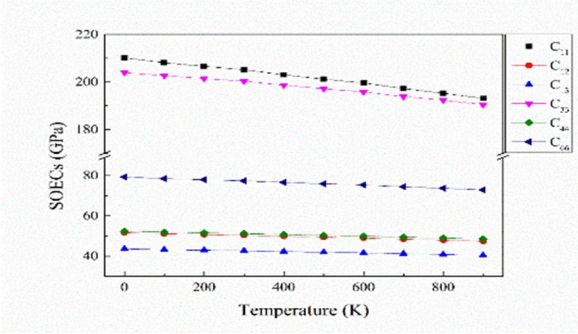

Fig. 1. Temperature dependence of SOECs

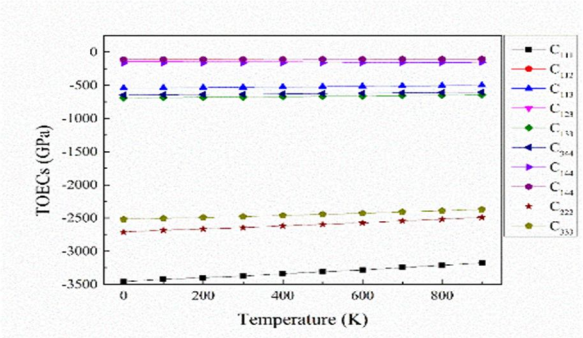

Fig. 2. Temperature dependence of TOECs

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From Fig. 1, it can be seen that with increase in temperature, the SOECs decrease while Fig. 2 depicts that with increase in temperature, the TOECs increase or remain linear. It can also be seen that the SOECs also fulfil the mechanical stability criteria[19] for hexagonal crystals, *i.e.* $C_{44}>0$, $C_{11}>|C_{12}|$, $(C_{11}+2C_{12})>2C_{13}$. This confirms the high mechanical stability of the alloy. Throughout the temperature range, C_{11} is always greater than C_{33} which indicates the atomic bonding to the nearest neighbour atoms along the (100) plane being stronger than that along the (001) plane of the crystal.

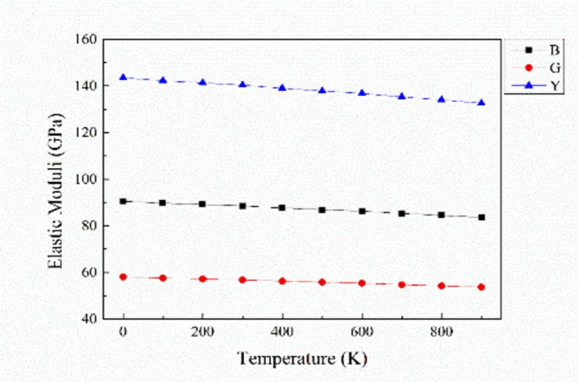

Fig. 3. Temperature dependence of bulk modulus (*B*), shear modulus (*G*) and Young's modulus

The bulk modulus (*B*), shear modulus (*G*), Young's modulus (*Y*) and Poisson's ratio have at different temperatures been computed using the Voigt-Reuss-Hill method[22] and are plotted in Fig. 3. While all of the elastic moduli decrease significantly with temperature, the Poisson's ratio is 0.2357 at room temperature (300K) and does not change significantly with temperature. The bulk modulus, shear modulus and Young's modulus at room temperature is 88.5 GPa, 56.79 GPa and 140.36 GPa respectively which are in good agreement with the values available in literature[5], [17].

The quasi-shear (V_{S1}), shear (V_{S2}), longitudinal (V_L) and Debye average (V_D) velocities at different angles with the unique axis in the temperature range 0-900K have been evaluated using the SOECs and density of the alloy and plotted in Fig. 4.

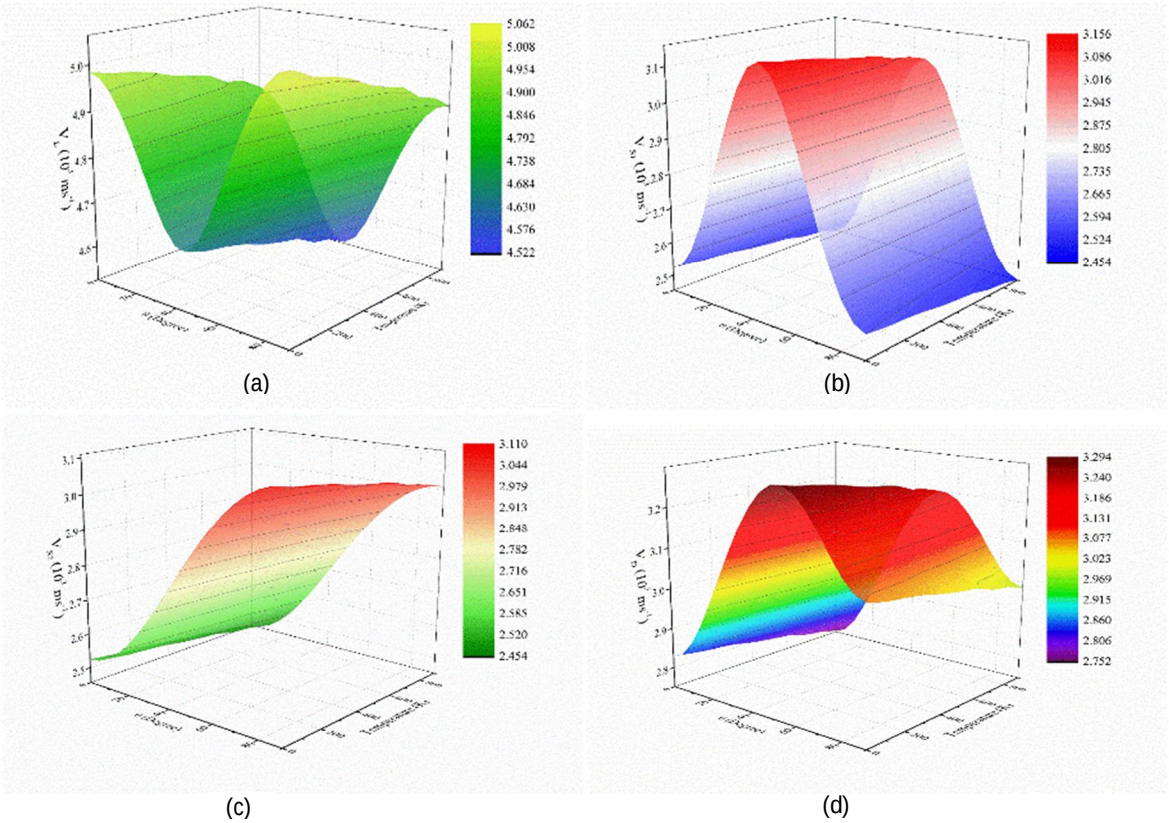

Fig. 4. Ultrasonic **(a)** longitudinal (V_L), **(b)** quasi-shear (V_{S1}) and **(c)** shear (V_{S2}) and **(d)** Debye average (V_D) velocities at different temperatures.

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The longitudinal wave velocity V_L decreases with increase in temperature but decreases with increase in angle θ up to 45° with the unique axis and start increasing again from 45-90°. The maximum with value of V_L is 5.06×10^3m/s at angle 90° with the unique axis at temperature 0K. The quasi-shear wave velocity V_{S1} also decreases with temperature but with have a maximum value of 3.16×10^3m/s at angle 45°. The shear velocity V_{S2} monotonically decreases with temperature while increases with angle θ. The Debye average velocity V_D shows similar nature to quasi-shear wave velocity with maximum value of 3.29×10^3m/s at 0 K temperature and angle θ=55°. The values of these ultrasonic velocities of Ti-Zr-Hf HCP alloy have not been found in literature but is in good agreement with studies of similar materials like Sc-Ti-Zr-Hf[16].

The Debye temperature (θ_D) decreases from 303.2K to 292.8K in temperature range of 0-900K. This shows that the Debye temperature does depend on temperature but the dependence is not very significant.

The heat capacity C_V and thermal energy density E_0 have been evaluated in temperature range of 0-900K by employing the Debye model and plotted in the Fig. 5.

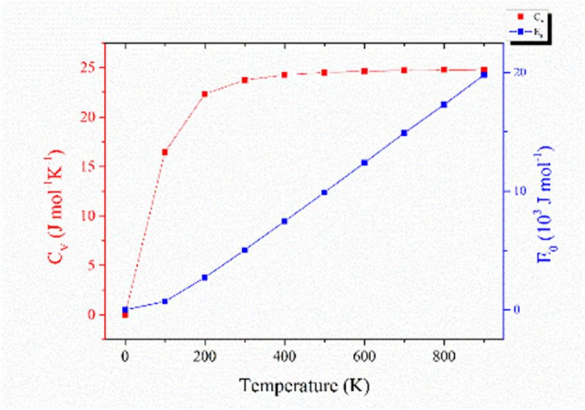

Fig. 5. Temperature dependence of Heat capacity (C_V) and thermal energy density (E_0)

From Fig. 5, it is evident that C_V increases with temperature but the dependence becomes less and less significant as the temperature increases making the plot plateau at higher temperature. The thermal energy density (E_0) monotonically increases with increase in temperature.

Thermal conductivity of a material is one of the important thermophysical properties and to evaluate it for the alloy, we used Eq. 1. The Grüneisen constant for thermal conductivity has been calculated with the help of Coefficient of thermal expansion α values available in the literature[17]. The dependence of thermal conductivity on temperature and direction in the crystal is plotted in the Fig. 6.

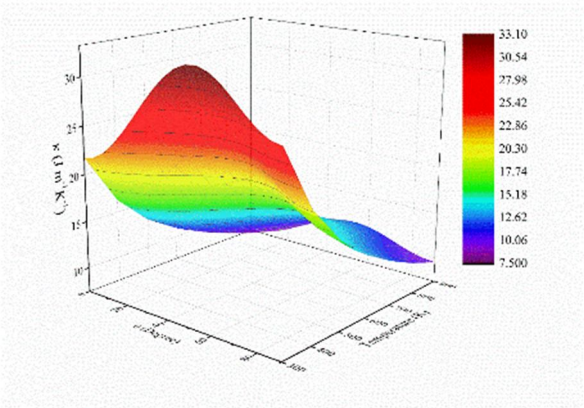

Fig. 6. Temperature and direction dependence (θ) of thermal conductivity (κ)

Thermal conductivity is 21.77 W/mK at 300K and 0° angle with unique axis and decreases with increase in temperature.

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The ultrasonic behaviour of HCP Ti-Zr-Hf alloy is major interest of the present study and ultrasonic attenuation is directly correlated to thermoelastic properties and nature of bond in a material. Therefore, the ultrasonic attenuation due to phonon-phonon interaction known as Akhiezer loss and due to thermos-relaxation mechanism have been estimated in temperature range of 300-900K using the formulation given in Eq. 2-4 and presented in Fig. 7.

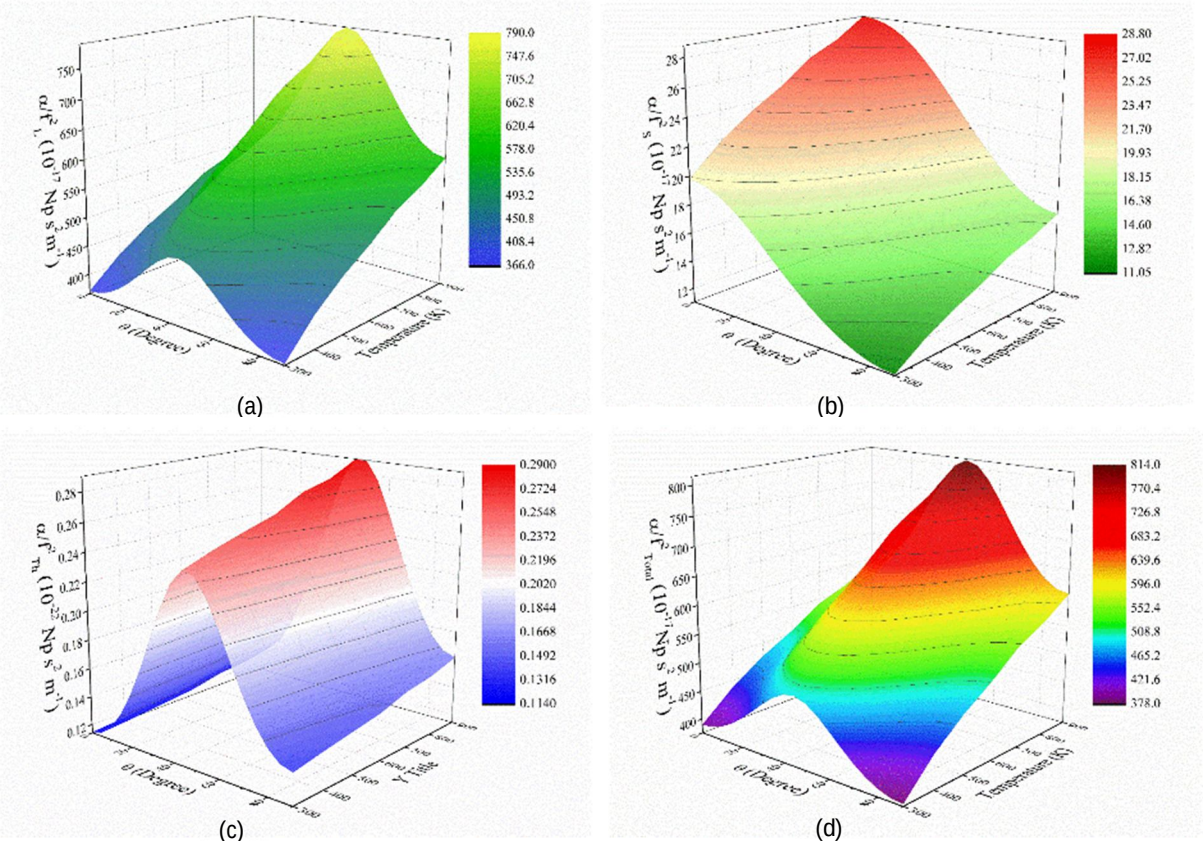

Fig. 7. Direction and temperature dependence of **(a)** longitudinal, **(b)** shear, **(c)** due to thermos-relaxation mechanism and **(d)** total ultrasonic attenuation

The ultrasonic attenuation in longitudinal mode $\left(\alpha/_{f^2}\right)_L$ shows highest value of 789.36×10^{-17} Np s^2/m at temperature 900K and angle (θ) 45° and lowest value of 367.46×10^{-17} Np s^2/m at 300K of temperature and 90° angle (θ) with unique axis. Akhiezer[26] already suggested that the attenuation due to phonon-phonon interaction dominates over other forms of attenuations including thermo-relaxation mechanism and the plots in Fig. 7 clearly exhibit this. The ultrasonic attenuation due to thermo-relaxation mechanism $\left(\alpha/_{f^2}\right)_{Th}$ is in range of 0.11×10^{-22} – 0.29×10^{-22} Np s^2/m in the temperature range of 300-900K.

The total attenuation $\left(\alpha/_{f^2}\right)_{Total}$ is sum of ultrasonic attenuation due to phonon-phonon interactions (longitudinal and shear modes) and due to thermo-relaxation mechanism. As attenuation in longitudinal mode dominates over shear mode and attenuation due to thermo-relaxation mechanism, the total attenuation shows similar nature with temperature and angle with unique axis.

IV. CONCLUSIONS

Based on the obtained results and discussion, the following conclusions have been drawn:

1) The results obtained are in good agreements with other studies available in literature. This confirms the significance and successful application of the Lennard-Jones potential approach.
2) The alloy shows strong mechanical stability.
3) The heat capacity follows Dulong-Petit law.
4) The ultrasonic attenuation in longitudinal mode is predominant over shear mode and thermoelastic attenuation.

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V. ACKNOWLEDGMENT

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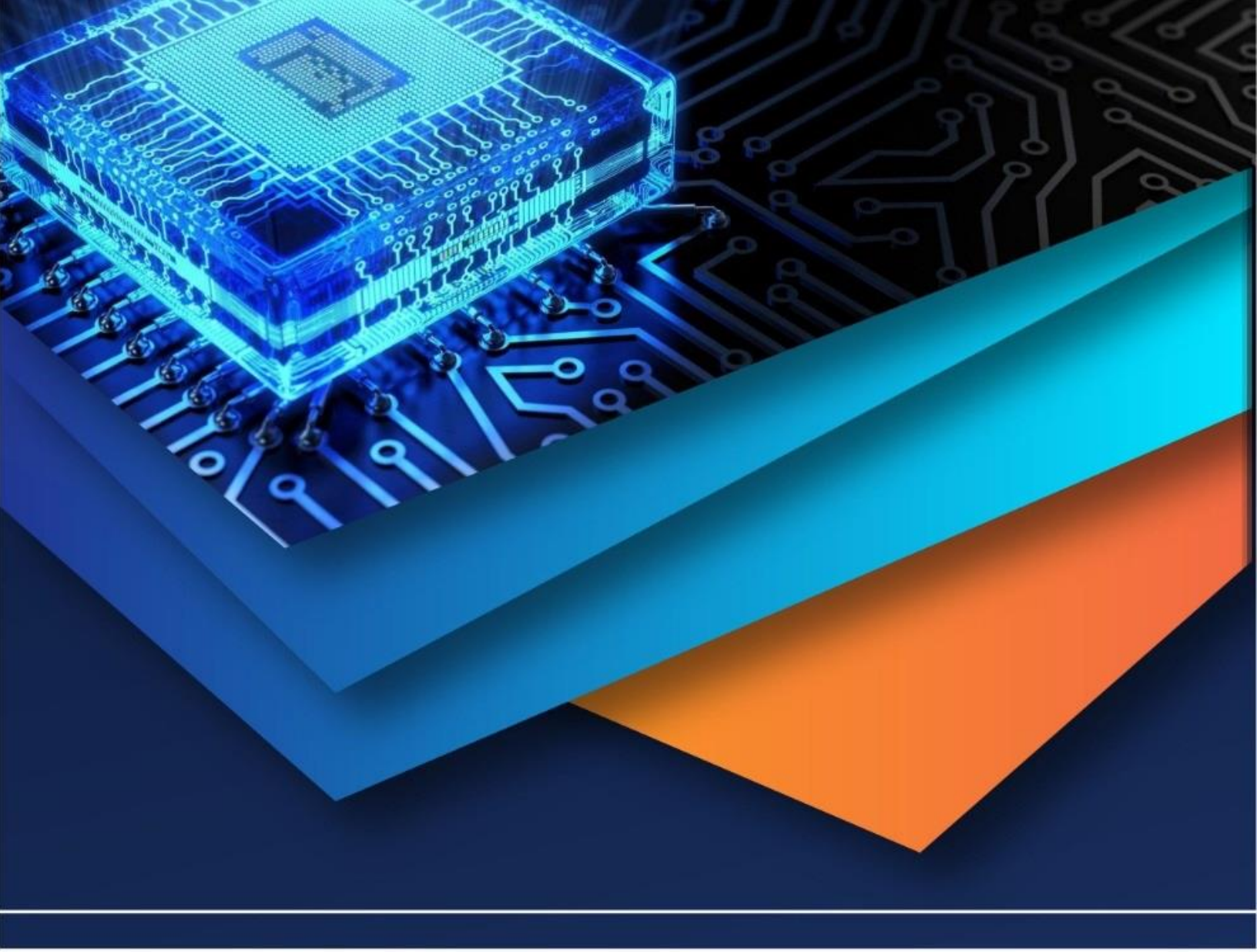

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