Elastic, Mechanical and Thermophysical Properties of HMo2 (H= Zr and Hf) Laves Phase Compounds

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ABSTRACT

Using the Lennard - Jones many body interactions potential technique, the elastic, mechanical, thermophysical, and ultrasonic characteristics of HMo2 (H= Zr and Hf) laves phase compounds were investigated. Other ultrasonic parameters are calculated using second-order elastic constants. Mechanical constants such as Young's modulus, bulk modulus, shear modulus, Poisson's ration, ductility, and anisotropy factor have also been calculated. Laves phase compounds satisfy the Born Criterion for mechanical stability since their Pugh's ratio (the ratio of bulk modulus to shear modulus) is smaller than 1.75, indicating that they are brittle. These ZrMo2 and HfMo2 ultrasonic velocities and thermal relaxation times are calculated using calculated elastic constants and lattice parameters under the same physical conditions. For the evaluation of anisotropic behaviour and thermophysical parameters, the orientation dependent ultrasonic velocities and thermal relaxation time were also examined. The obtained results are evaluated in order to understand more about the properties of laves phase compounds.

Keywords : Laves Phase Compounds, Ultrasonic Properties, Elastic Properties

I. INTRODUCTION

The laves phases of intermetallic compounds have been given a lot of thought because of their excellent physical and chemical features, [1–2]. Laves phases have been investigated for a variety of applications, including high-temperature structural materials with excellent corrosion and oxidation resistance, hydrogen storage materials and superconducting materials, and resistance superconducting materials [3–5] because of its refractory character, molybdenum (MO) and related alloys are widely utilised in a

variety of applications where severe environment resistance is required, such as in caustic chemicals. Zirconium is primarily utilised as a container for nuclear fuel in light water reactors in the nuclear power sector, owing to its low neutron absorption crosssection [6]. Mo alloys are intermetallic compounds in general. Since the discovery of intermetallic compounds with intriguing properties such as polymorphism and unusual magnetic and electrical properties, the leaves phase has been a popular topic of discussion [7–9]. Magnetostrictiv materials and high temperature structural materials

are significant for applications in hydrogen storage materials; superconducting materials and enormous are related to magnetostrictiv materials. At high temperatures, the phases usually exhibit particular magnetic properties as well as high strength and oxidation resistance. ZrMo2 is an another Zr-compound that is an important nuclear structural material and cladding material for reactor nuclear fuels [10, 11].

We worked very hard in this research work to establish relationship between thermophysical and microstructural properties forHMo2(Hf and Zr)

compounds, which will aid in understanding the mechanical behaviour of hexagonally structured HMo2 (X = Hf and Zr) compounds and play an important role in the diagram of a manufacturing apparatus with useful physical properties under moderate working conditions. Thermal relaxation time and ultrasonic velocity for hexagonally structured HMo2 (X = Hf and Zr) compounds were considered for it though. For hexagonally structured HMo2 (X = Hf and Zr) compounds, the bulk modulus (B), shear modulus (G), Young's modulus (Y), Pugh's ratio (B / G), and Poisson's ratio were computed and discussed.

II. METHODS AND MATERIAL

The Lenard Jones interaction potential methods will be used for the evaluation of SOECs and TOECs in this investigation. The partial derivatives of the thermodynamic potential of the medium constrained to finite deformation, as well as mathematically expressed by subsequent expression such [12, 13], are a generalised characterization of the n th order elastic coefficient.

The partial derivatives of the medium constrained finite deformation's thermodynamic potential, as well as following expressions like are a universal description of the nth order elastic constant. [25, 26],

$$C_{ijklmn\ldots} = \frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn \cdots}} \tag{1}$$

F refers for free energy density, whereas η_{ij} stands for Lagrangian strain component tensor. Taylor series expansion η can be used to extend F in terms of strain:

$$F = \sum_{n=0}^{\infty} F_n = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn \cdots}} \right) \eta_{ij} \eta_{kl} \eta_{mn} \cdots \tag{2}$$

As a function, the free energy density is represented as:

$$F_2 + F_3 = \frac{1}{2!} C_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{3!} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} \tag{3}$$

The basis vectors are $a_1 = a \left(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0 \right)$, $a_2 = a(0,1,0)$ and $a_3 = a(0,0,c)$ in cartesian coordinates axis are used to make hexagonal compounds. The unit cell lattice parameters are a and c. The unit cell of an HCP compound is made of two non-equivalent atoms: six in the basal plane and three in the upper and lower planes. As a result, both the first and second neighborhood have six atoms. The location vectors among those two types of atoms are $r_1 = a(0,0,0)$ and $r_2 = \left(\frac{a}{2\sqrt{3}}, \frac{a}{2}, \frac{c}{2} \right)$.

$$\varphi(r) = -\frac{a_0}{r^m} + \frac{b_0}{r^n} \tag{4}$$

Where a0 and b0 are constants, m and n are integers, and r is the atom distance. Our earlier studies used the interaction potential model to compute six SOECs and ten TOECs of the hexagonal compound, as well as formulations of elastic constants.

Voigt and Reuss' techniques [14, 15] were used to compute the bulk and shear moduli. The Voigt and Reuss techniques, respectively, used unchanging stress and unchangeable strain computations. Furthermore, the average values of both approaches were utilised to determine the resulting values of B and G [16] using Hill's techniques. The Young's modulus and Poisson's ratio are calculated using bulk and shear modulus values, respectively [17, 18]. For the evaluation of Y, B, and Gand, the following expressions were performed.

$$
\left.\begin{array}{l}
M = C_{11} + C_{12} + 2C_{33} - 4C_{13}; \mathrm{C}^2 = (C_{11} + C_{12})C_{33} - 4C_{13} + C^2{}_{13}; \\
B_R = \frac{C^2}{M}; \mathrm{B}_V = \frac{2(C_{11}+C_{12})+4C_{13}+C_{33}}{9}; \\
G_V = \frac{M+12(C_{44}+C_{66})}{30}; \mathrm{G}_R = \frac{5C^2 C_{44}C_{66}}{2[3B_V C_{44}C_{66}+C^2(C_{44}+C_{66})]}; \\
Y = \frac{9GB}{G+3B}; \quad \mathrm{B} = \frac{B_V+B_R}{2}; \quad \mathrm{G} = \frac{G_V+G_R}{2}; \sigma = \frac{3\mathrm{B}-2\mathrm{G}}{2(3\mathrm{B}+G)}
\end{array}\right\}
\tag{5}
$$

Because the velocity of ultrasonic waves is primarily determined by SOECs and density, the anisotropic and mechanical properties of hcp structured materials are highly associated with ultrasonic velocity. In a hexagonal structured compound, there are three types of ultrasonic velocities based on the mode of vibration. Wave velocities of the first longitudinal V_L and second shear (V_{S1}, V_{S2}) waves.[19,20] The following equations describe ultrasonic velocities for hexagonal structured compounds based on the angle between the direction of propagation and the z-axis:

$$
V_L = \sqrt{\frac{C_{33}}{\rho}}
\tag{6}
$$

$$
V_S = \sqrt{\frac{C_{44}}{\rho}}
\tag{7}
$$

where, V_L, V_s are the longitudinal, quasi-shear, and shear wave velocities, respectively.

$$
V_D = \left[\frac{1}{3}\left(\frac{1}{V_L^3} + \frac{1}{V_{s1}^3} + \frac{1}{V_{32}^3}\right)\right]^{-1/3}
\tag{8}
$$

At low temperatures (less than 100K), the electron-phonon interaction dominates ultrasonic wave attenuation mechanisms. The mean free path of electrons is the same as the mean free path of acoustical phonons at this temperature regime. As a result, there is a significant probability of interaction between free electrons and acoustic phonons [20]. The following is the mathematical formula for ultrasonic attenuation for longitudinal ($\acute{\alpha}$)Long and shear waves ($\acute{\alpha}$)Shear caused by energy loss due to electron-phonon interaction:

$$
\alpha_{long} = \frac{2\pi^2 f^2}{\rho V_l^3}\left(\frac{4}{3}\eta_e + \chi\right)
\tag{9}
$$

$$
\alpha_{shear} = \frac{2\pi^2 f^2}{\rho V_S^3}\eta_e
\tag{10}
$$

where 'ρ' is the density of nanostructured compound, 'f' is the frequency of the ultrasonic wave, 'η_e' is the electron viscosity and 'χ' is the compressional viscosity (which is zero in present case),

At higher temperatures, the two dominant processes are p-p interaction (Akhieser's type loss) and thermoelastic loss, both of which are significant for ultrasonic wave attenuation. The following equation describes the attenuation due to Akhieser's loss:

$$(\alpha/f^2)_{Akh} = \frac{4\pi^2\tau E_0(D/3)}{2\rho V^3} \tag{11}$$

Here, f represents the frequency of the ultrasonic wave; E_0 is the thermal energy density.
. The thermoelastic loss $(\alpha/f^2)_{Th}$ is considered by the subsequent equation:

$$(\alpha/f^2)_{Th} = 4\pi^2 < \gamma_i^j >^2 \frac{kT}{2\rho V_L^5} \tag{12}$$

The total attenuation is specified by the subsequent equation as:

$$(\alpha/f^2)_{Total} = (\alpha/f^2)_{Th} + (\alpha/f^2)_L + (\alpha/f^2)_S \tag{13}$$

Wherever $(\alpha/f^2)_{Th}$ is the thermoelastic loss, $(\alpha/f^2)_L$ and $(\alpha/f^2)_S$ are the ultrasonic attenuation coefficient for the longitudinal wave and shear wave correspondingly.

III. RESULTS AND DISCUSSION

3.1 Higher order elastic constants

We used an interaction potential approach to calculate the elastic constants (six SOECs and ten TOECs) in this study. For HfMo2 and ZrMo2, the lattice parameters 'a' (basal plane parameter) and 'p' (axial ratio) are 5.417, 5.373 and 1.591, 1.599, respectively [21]. For the leaves phase compound, the chosen values of m and n are 6 and 7. For HfMo2 and ZrMo2 compounds, b_0 values are 4.62x10-62 erg cm7 and 4.66x10-62 erg cm7, respectively. Table 1 shows the SOECs and TOECs estimated for various leaves phase compounds at room temperature.

Table1. SOECs, TOECs and bulk modulus (inGPa) at room temperature.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B
HfMo2	302	74	61	284	74	118	142
HfMo2[16]	301.3	154.4	157.9	297.9	46.3	73.4	---
ZrMo2	281	69	56	259	68	110	131
ZrMo2[16]	281.2	150.5	153.7	269.1	37.7	65.6	---

	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{344}	C_{144}	C_{155}	C_{222}	C_{333}
HfMo2	-4933	-782	-158	-201	-960	-900	-234	-156	-3903	-3452
ZrMo2	-4589	-727	-145	-185	-875	-820	-216	-144	-3613	-3116

HfMo2 and ZrMo2 had the higher elastic constant values, which are important for the material, as these are associated with the stiffness parameter. SOECs are used to determine the associated parameters. Evidently, for steady of the hexagonal compound, they would satisfy the renowned Born- Huang's stability norms [19, 20] i.e.$C_{11}- |C_{12}| > 0$, $(C_{11}+C_{12}) C_{33}- 2C^2_{13}> 0$, $C_{11}> 0$ and $C_{44} > 0$. In Table 1, It is evident that the values of above elastic constant are positive too satisfies Born-Huang's mechanical stability criteria and therefore totally these compounds are mechanically stable. The evaluated coefficients of C12, C13 and C66 are some differ than other results of theoretical [21] for HfMo2 and ZrMo2 compound. Essentially Turkdal, et al. [21] has been theoretically evaluated by DFT investigations, which is rather differ from reported method. While found order of SOECs are of the similar as specified in Table 1[21]. Comparative magnitude of elastic constant C11, C33, and C44 are well obtainable by our approach. Thus, there is respectable agreement between the presented and the informed values which is correlated with elastic constants. Therefore, our theoretical methodology is well justified for the evaluation of SOECs of hexagonal arranged compounds. We present the calculated values of TOECs in table 1. The negative values of TOECs indicate a negative strain in the solid. Negative TOECs appear in the previous paper on hexagonal structure material. Therefore, this applied theory for valuation of higher order elastic constants is justified [22, 23]. Hence, the applied theory for the valuation of the elastic constants is justified.

Table 2. Voigt–Reuss, constants (M and $C^{2)}$,Bulk modulus ($x10^{10}Nm^{-2}$), Shear Modulus ($x10^{10}Nm^{-2}$), Young's Modulus ($x10^{10}Nm^{-2}$), Poisson,s Ratio, Pugh,s Ratio for HfMo2 and ZrMo2 compound.

	M	C2	Br	Bv	Gr	Gv	Y	B/G	G/B	σ
HfMo2	700	110261	158	142	97	100	242	1.52	0.65	0.231
ZrMo2	644	93562	145	131	105	93	239	1.40	0.71	0.211

It is found that the value of B, Y, and G of ZrMo2 leaves phase compound are smaller than HfMo2 leaves phase compound. Thus ZrMo2 have little Stiffness and bonding with respect to HfMo2 leaves phase compound. B/G and 'σ' are the measure of brittleness and ductility of solid. If σ= ≤0.26 and B/G = ≤1.75, the solid is generally brittle, otherwise it is ductile in nature [16, 24] . Our finding of lower values of B/G and σ compared to their critical values indicates that HfMo2and ZrMo2 is brittle in nature at room temperature. It is well known that for stable and elastic material the value of σ should be less than 0.5. The values of 'σ' evaluated for HfMo2 and ZrMo2 are smaller than its critical value. It indicates that HfMo2 and ZrMo2 is stable corresponding to shear. The compressibility, hardness, ductility, toughness, brittleness and bonding nature of the leaves phase compounds are too well connected with the SOECs.

3.2 Ultrasonic Velocity andUltrasonic allied parameters

In present analysis, we have correlated the mechanical and isotropic behavior of the hexagonal compound with ultrasonic velocity. We have calculated V_L, V_S, V_D and $τ$ for leaves phase compounds. The angular dependence Figures 1-4. The angles are measured form the z-axis of the crystal. Form figs. 1 and 2 velocities VL and VS1 of HfMo2 and ZrMo2 have minima and maxima at 450 respectively. In Figure 3, we find that VS2 increases with angle form the z- axis. The irregular behavior of orientation dependent velocity is due to combined effect of SOECs and density. The nature of the orientation dependent velocity curves in this work is similar to nature of
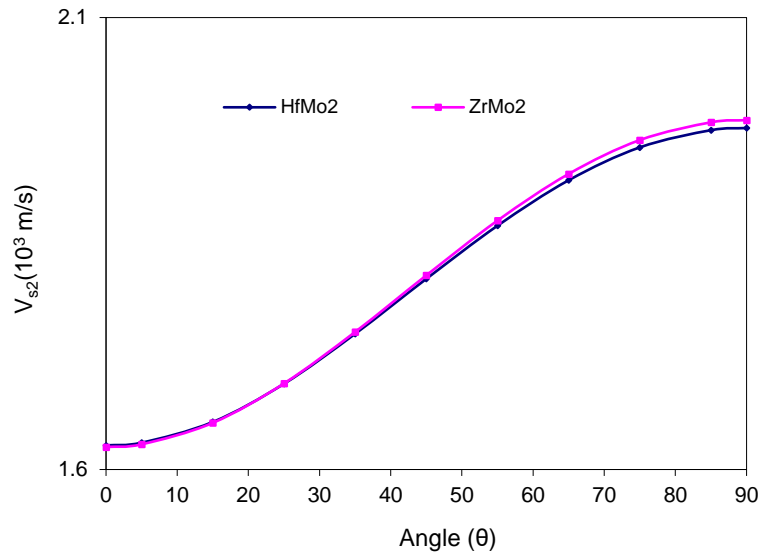
orientation dependent velocity curve found for other hexagonal type's material [22, 23]. Thus, the angle dependence of the velocities in leaves phase compounds is justified.
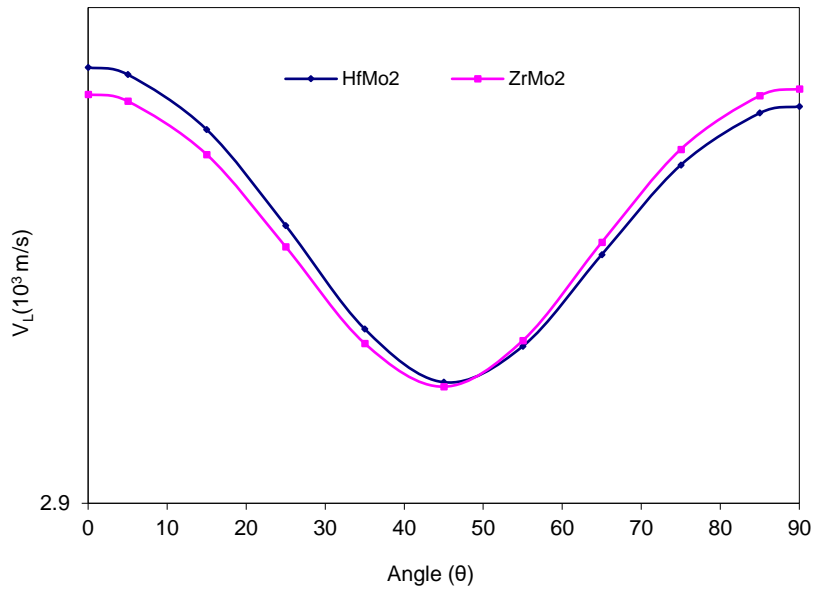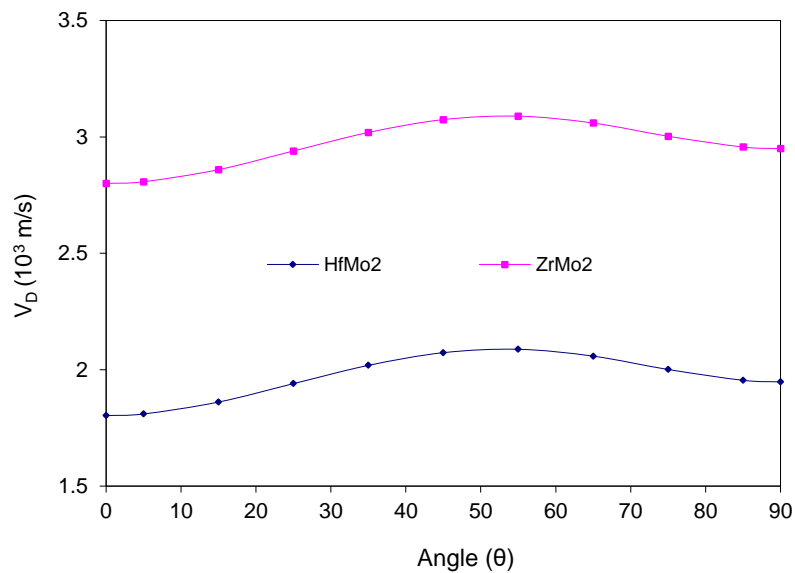

Fig. 1. V_L vs Theta with unique axis of crystal
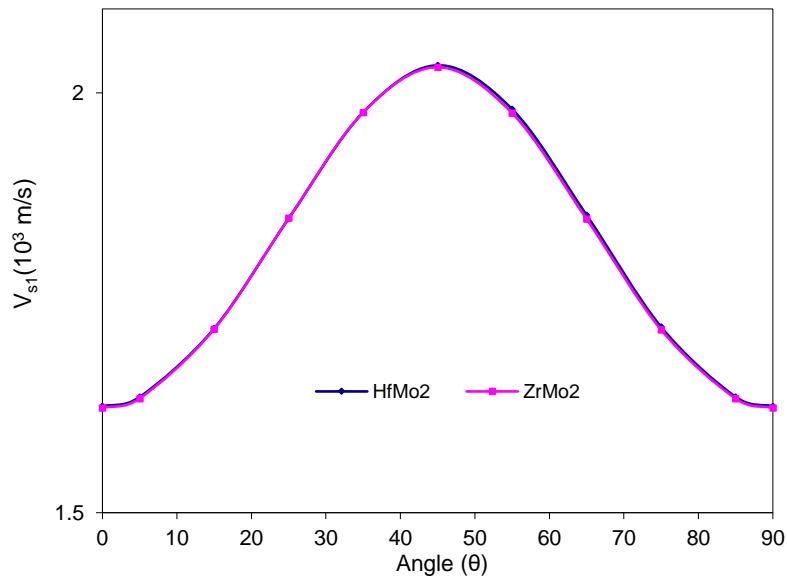
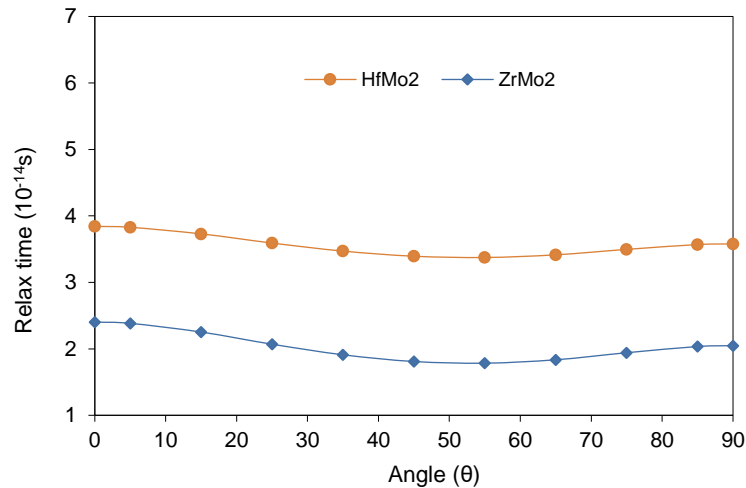**Fig. 2.** V_{S1} vs Theta with unique axis of crystal

Fig. 3. V$_{S2}$ vs Theta with unique axis of crystal

Fig. 4. V$_D$ vs Theta with unique axis of crystal

Figure 4 shows the variation of Debye average velocity (VD) with the angle made with the z- axis of the crystal. It is clear that VD increases with the angle and reaches maximum at 550 for both transition metal disilicides. As the calculation of VD involves the velocities VL, VS1 and VS2 [25, 26], It is understandable that the variation of Debye average velocity is affected by the fundamental ultrasonic velocities. Maximum value of VD at 55° is due to a significant increase in pure shear and longitudinal wave velocities and a decrease in quasi-shear wave velocity. It may be determined that the average sound wave velocity is a maximum when a sound wave travels at 550 angles with the z- axis of this crystal.

Fig. 5. Relaxation time vs Theta with unique axis of crystal axis

Figures 5 show a plot of the calculated thermal relaxation time 'τ' with the orientation dependent. Angle dependent 'τ' curves track the reciprocal nature of V_D as $\tau \propto 3K / C_V V_D^2$ .. It is 2 *D* clear that thermal relaxation time for leaves phase compounds is mainly affected by 'k'. Thermal relaxation time for hexagonal structured material is of order at picoseconds [22, 27]. Therefore, the calculated 'τ' explains the hexagonal structure of leaves phase compounds. The lowest value of θ' = 55⁰ denotes that the re-establishment time for equilibrium for wave propagation along τ' distribution of thermal phonons will be minimum for propagation of wave along this direction.

IV. CONCLUSIONS

Based on the discussion above, it is important to note that the notion of using a simple interaction potential technique to calculate higher-order elastic coefficients for hexagonally organised leaves phase compounds remains valid. The elastic constants must satisfy the well-known Born's stability criterion for superconducting leaves phase compounds to be stable. The ductile nature of superconducting compounds is confirmed by the Pugh's ratio. The "τ" is determined to be of the order of picoseconds for HfMo2 and ZrMo2 leaves phase complexes, defending their hexagonal structure. Because "τ" has the smallest value along = 55⁰ at all temperatures, the duration required for the re-establishment of phonon symmetry spreading will be the shortest for wave propagation in this direction. HfMo2 leaves phase compound has a better mechanical behaviour than ZrMo2 leaves phase compound.

Processing and non-destructive characterisation of leaves phase compounds could benefit from this research. These findings will serve as a foundation for further research into the major thermophysical features of additional leaves phase compounds.

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Cite this article as :