Theoretical Investigations of Elastic Constants and Ultrasonic Wave Propagation in Co_3- X (X = Mo, Nb,Ta) Alloys

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Abstract: ***Elastic constants and ultrasonic velocity are well connected to the micro structural and mechanical properties of materials. In the present paper the ultrasonic properties of hexagonal closed packed structured alloys Co_3Mo, Co_3Nb and Co_3Ta were investigated. For the study of ultrasonic properties, the second order elastic constants for these alloys were computed using the Lennard - Jones potentials. The ultrasonic velocities V_1(longitudinal) , V_2(quasi shear), and V_3(pure shear) for these alloys were calculated .These angle dependant velocities V_1 and V_2 showed a minima and maxima respectively, when the ultrasonic wave travelled ,making an angle of 45^0 with unique axis of crystal. Also, the Debye average sound velocity for these alloys was found to exhibit maxima at an angle 55^0 with unique axis of crystal. The pure shear wave velocity V_3 was found to increase with the angle. The inconsistent behaviour of these angle dependant ultrasonic velocities could be attributed to the effect of the second order elastic constants of these alloys. These ultrasonic properties are useful for characterization of alloys and to determine their suitability for mechanical and industrial applications.***

1. Introduction

Ultrasonics studies of materials are a widely used tool for various material studies and characterization. Ultrasonic velocity and other parameters are well connected to the micro structural and mechanical properties of the materials. Ultrasonic properties of various alloys, compounds, metals have been widely investigated as versatile tool in studying the inherent properties and internal structure of solids[1-4].Ultrasonic properties offer the possibility to detect and characterise the micro structural properties as well as the flaws in the materials, control the materials behaviour based on physical mechanism and to predict future performance of materials. Wave propagation and velocity is a vital parameter in ultrasonic characterisation and can be used to obtain information about crystallographic texture .The ultrasonic velocity is directly related to elastic constants by relation $V=\sqrt{\frac{C}{\rho}}$, where C and ρ are elastic constant and density of material respectively.

The elastic constants of material provide valuable information about nature of atomic bonding forces and related hardness of the material [5-6].From electronic band structures, Co was found to be stable in fcc structure[8]. But, ion –beam mixing studies show that Co could also possess hcp structure[9-10]. Zhang et al, had studied Ni-X(X= Mo, Nb,Ta) alloys using solid state reaction method[11-12]. Ni-R(R= Mo, Nb,Ta) alloys have been studied using their elastic constants.[19] Since Co is known to possess nearly same mass number and lattice parameters as Ni, in the present paper, ultrasonic properties like angle dependant sound velocity and second order elastic constants for Co-X(X= Mo, Nb,Ta) alloys are evaluated and discussed.

Theory

The second order elastic constants (C_{ij}) of the material are given by

$$C_{ij} = \frac{\partial^2 U}{\partial_{ei}\partial_{ej}} \text{ , i or j =1--6 (1)}$$

U is the elastic energy density, $e_i = e_j$ is the component of strain tensor. There exist six second order elastic constants for the hexagonal closed packed structured materials[13-14] given by

$C_{11} = 24.1p^4 C'$, $C_{12} = 5.91\, p^4 C'$, $C_{13} = 1.925\, p^6\, C'$, $C_{33} = 3.46p^8\, C'$, $C_{44} = 2.30\, p^4 C'$, $C_{66} = 9.85\, p^4 C'$ (2)

Where $C' = \chi a/p^5$, $\chi = (1/8)[\{nb_0(n-m)\}/(a^{n+4})$], m, n = integers; b_0 = Lennard-Jones parameter, p = c/a : axial ratio ; a and c are the unit cell parameters.

As the ultrasonic velocity is related to second order elastic constants, the anisotropic behaviour of the material alloy can be understood by knowing these velocities [14]. There are three types of velocities:- longitudinal , quasi-shear , and shear, depending on the mode of atomic vibrations [15]. These velocities vary with the direction of propagation of wave with respect to the unique axis of hexagonal crystal. The ultrasonic velocities as function of angle between direction of propagation and unique axis of hexagonal crystal are given as in ref [16]

$$V_1^2 = \{C_{33}\cos^2\theta + C_{11}\sin^2\theta + C_{44} + \{[C_{11}\sin^2\theta - C_{33}\cos^2\theta + C_{44}(\cos^2\theta - \sin^2\theta)]^2 + 4\cos^2\theta\sin^2\theta\,(C_{13}+C_{44})^2\}^{1/2}\}/2\rho \quad (3)$$

$$V_2^2 = \{C_{33}\cos^2\theta + C_{11}\sin^2\theta + C_{44} - \{[C_{11}\sin^2\theta - C_{33}\cos^2\theta + C_{44}(\cos^2\theta - \sin^2\theta)]^2 + 4\cos^2\theta\sin^2\theta\,(C_{13}+C_{44})^2\}^{1/2}\}/2\rho \quad (4)$$

$$V_3^2 = \{C_{44}(\cos^2\theta + C_{66}\sin^2\theta\}/\rho \quad (5)$$

Where V_1 , V_2 , V_3 are longitudinal, quasi-shear, and pure shear wave ultrasonic velocities. ρ and Θ represent the density of material and angle with the unique axis of the crystal respectively. The Debye average velocity V_D is given by

$$V_D = \left\{\frac{1}{3}\left(\frac{1}{V_1^3}+\frac{1}{V_2^3}+\frac{1}{V_3^3}\right)\right\}^{-\frac{1}{3}} \quad (6)$$

The Bulk modulus of these alloys can be calculated using the formula as in ref [16]

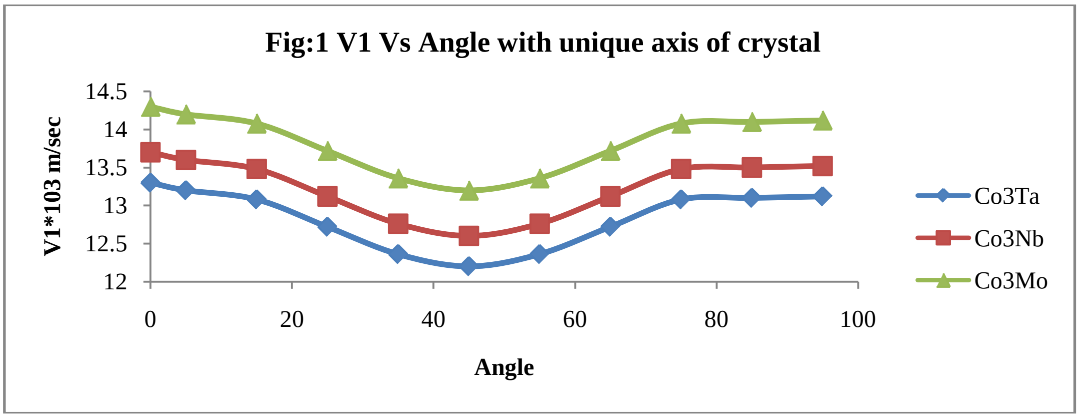
$$B = \frac{2}{9}\left(C_{11}+C_{12}+2C_{13}+\frac{C_{33}}{2}\right) \quad (7)$$

Table 1: Second order elastic constants and bulk modulus (B) for Co_3-X(X= Mo,Nb,Ta) alloy at room temperature.

Alloy	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	Calculated bulk modulus $B*10^{10}\ Nm^{-2}$	experimental bulk modulus. ref[17] $B*10^{10}\ Nm^{-2}$
Co_3Mo	35.4	8.74	7.55	35.4	8.86	13.4	16.42	17.16
Co_3Nb	31.4	8.59	6.22	33.3	8.38	12.0	15.30	15.08
Co_3Ta	30.1	7.23	6.10	30.6	8.09	11.5	15.02	14.35

2. Result and Discussion

The unit cell parameters a , for Co_3Mo , Co_3Nb, Co_3Ta are 2.574 A^0 , 2.604 A^0, 2.594 A^0 and the axial ratios p are 1.632, 1.629, 1.629, respectively as in ref[12]. The evaluated value of the Lennard-Jones parameter b_0 , for these alloys (for m=6, n=7) is 3.632 * 10^{-65} erg-cm^7 . The second order elastic constants using eq (2) and bulk modulus of elasticity using eq (7) are given in table.1. There exists a good agreement between the theoretically calculated values and the experimentally deduced values of the bulk modulus of elasticity for these alloys.



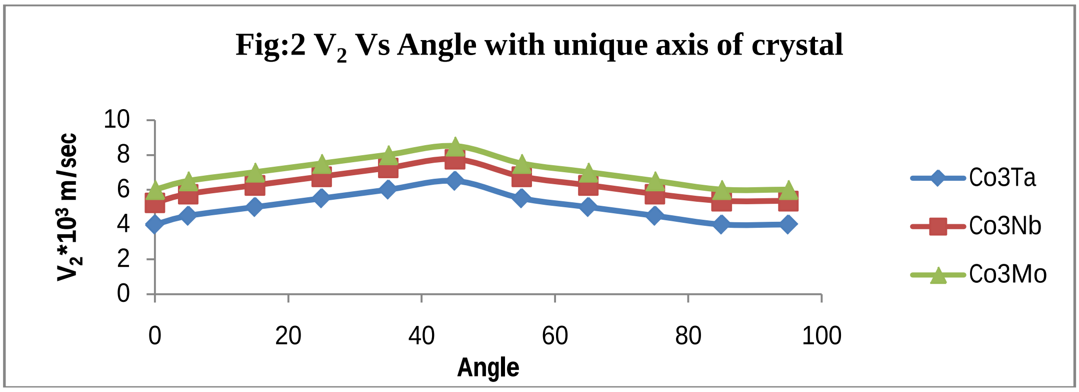


Fig:3 V_3 Vs Angle with the unique axis of crystal

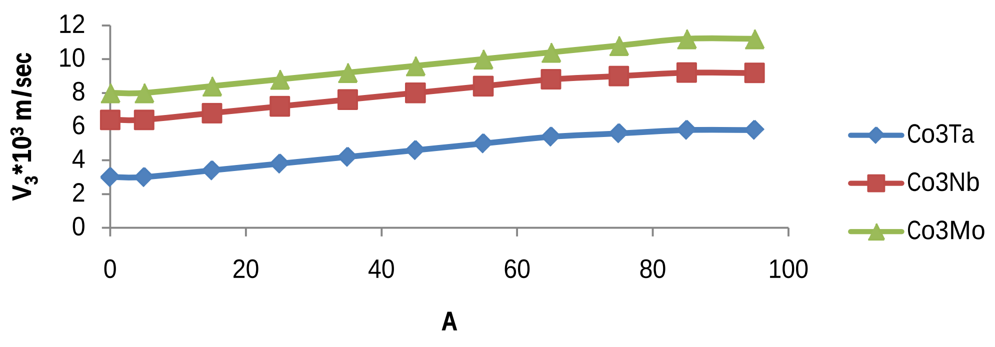
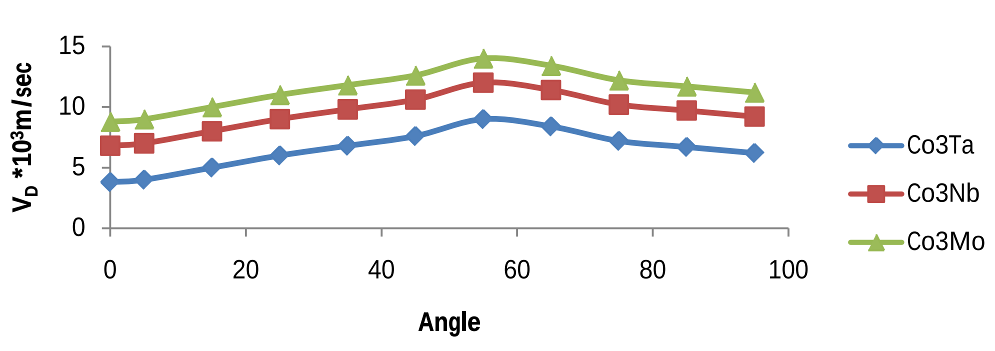


Fig:4 V_D Vs Angle with unique axis of crystal



The orientation dependant ultrasonic velocities for these alloys are given graphically in figure 1-4. It is found that the velocities V_1 and V_2 have minima and maxima respectively for an angle of 45^0 with the unique axis of the hexagonal crystal. Velocity V_3 goes on increasing as angle Ɵ with unique axis increases. The magnitude of longitudinal velocity along (001) direction is largest for Co_3-Mo alloy as it has highest C_{33} value. The shear velocities V_2 and V_3 have nearly same magnitude at $Ɵ = 0^0$ and different at other angles. The Debye average velocity V_D has maxima at angle $Ɵ = 55^0$, which is due to increase in longitudinal and pure shear wave velocity and decrease in quasi-shear wave velocity. As Co_3-Mo alloy has the maximum velocity, it has less defects in crystal structure, is supposed to be more ductile and stable alloy.

3. Conclusion

The present theoretical work to calculate second order elastic constants and the bulk modulus of elasticity is nearly accurate, which is evident from good agreement between theoretical and experimental values. The ultrasonic velocity is influenced by the elastic constants and density of material, and the direction of propagation of the wave. The (001) direction is the direction of symmetry as quasi-shear and shear waves have nearly same velocity magnitude along it. The high elastic constant and velocity for Co_3-Mo alloy makes it more suitable for industrial applications as compared to other chosen alloys. The inconsistent behaviour of these angle dependant ultrasonic velocities could be attributed to the effect of the second order elastic constants of these alloys. These ultrasonic properties are useful for characterization of alloys and to determine their suitability for mechanical and industrial applications.

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