

Table3 Relationship between atomic weights and velocities of $[Li_{0.5+x} Sb_x Fe_{2.5-2x}] O_4$ ferrites

Sl.no	X	V_l/ρ	V_s/ρ	V_m (m/s)	θ_D (K)
1	0.0	1.28	0.71	3701	504
2	0.1	1.34	0.74	3614	479
3	0.2	1.31	0.70	3423	453
4	0.3	1.27	0.67	3290	433
5	0.4	1.11	0.59	2986	397
6	0.5	1.09	0.59	3006	400

A plot of average sound velocity (V_m) against Debye temperature is shown in Fig. 1. It is interesting to note from the figure that the average sound velocity decreases linearly with the Debye temperature finally slightly/slight increased at $x=0.5$. This behavior clearly indicates direct relationship between the acoustic parameter (average sound velocity) and the important thermodynamic parameter (Debye temperature).

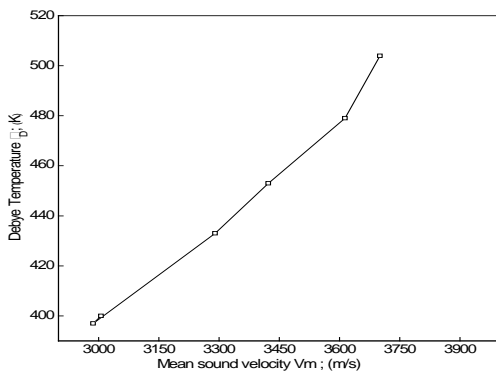


Fig 1. Variation of average sound velocity (V_m) with Debye temperature (θ_D) for antimony substituted lithium ferrites.

The elastic moduli can also be evaluated from IR study has been developed by Modi et al [7-9]. In the present study the elastic moduli were calculated only for $x=0.0$ and other samples are not performed due to lack of cation distribution from Mössbauer spectrometer for calculating force constants. The force constant is a second derivative of potential energy with respect to the site radius (R_A and R_B), the other independent parameter being kept constant, for tetrahedral site (K_t) and octahedral site (K_o), were calculated employing the method substituted by Waldron [10].

According to Waldron the force constants, K_t and K_o for respective sites are given by:

$$K_t = 7.62 \times M_A \times v_1^2 \times 10^{-7} \text{ N/m} \quad (12)$$

$$K_o = 10.62 \times M_{B/2} \times v_2^2 \times 10^{-7} \text{ N/m} \quad (13)$$

Where M_A and M_B are the molecular weights of cation on A-site and B-site calculated cation distribution ($Fe^{3+}[Li_{0.5} Fe_{2.5}]$ [11] for pure lithium ferrite ($x=0$). From the Fig.2 the primary absorption band (ν_1) is 582 cm^{-1} and the secondary absorption band (ν_2) is 476 cm^{-1} . the average force constant is listed in Table 4. The elastic moduli can be evaluated using the following relation [12,13].

$$\text{Bulk modulus (K)} = \frac{1}{3}(C_{11} + C_{12}) = L - \frac{4}{3}G \quad (14)$$

Where C_{11} and C_{12} are the stiffness constant. But according to Waldron [10] for isotropic materials with cubic symmetry like spinel ferrites and garnets $C_{11} \approx C_{12}$. Therefore, $K = C_{11}$. Also, the force constant(K) is a product of lattice (a) and stiffness constant (C_{11}) i.e. $K = aC_{11}$ [14]. And K is also average force constant ($K = (K_t + K_o)/2$). The value of lattice constant obtained from X-ray diffraction analysis is 8.333 \AA . The other elastic moduli of the ferrite specimens are calculated using following formulae [15,16] for a cubic lattice:

$$\text{Stiff constant (C}_{12}) = \frac{\sigma C_{11}}{(1-\sigma)} \quad (15)$$

$$\text{Rigidity modulus (G)} = \frac{E}{2(1+\sigma)} \quad (16)$$

$$\text{Young's modulus (E)} = 2(1 + \sigma) \rho(V_s)^2 \text{ or}$$

$$(E) = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{C_{11} + C_{12}} \quad (17)$$

$$\text{Poisson's ratio } (\sigma) = \frac{3K - 2G}{6K + 2G} \quad (18)$$

We have determined the value of longitudinal elastic wave velocity (V_l) using the formula suggested by Waldron [10],

$$V_l = \left(\frac{C_{11}}{\rho} \right)^{1/2} \text{ and the transverse elastic wave velocity}$$

(V_s) by general approximation [16,17] $V_l = 3^{1/2} V_s$. The values of V_l and V_s are further used to calculate the mean velocity and Debye temperature of the ferrite specimen using the following formula [18]:

$$\text{Mean elastic Wave velocity (V}_m) = \left[\frac{v_1^3 + v_s^3}{2v_1^3 + v_s^3} \right]^{1/3} \quad (19)$$

$$\text{Debye temperature } (\theta_D) = \frac{h}{k} \left[\frac{3N_A}{4\pi V_A} \right]^{1/3} \quad (20)$$

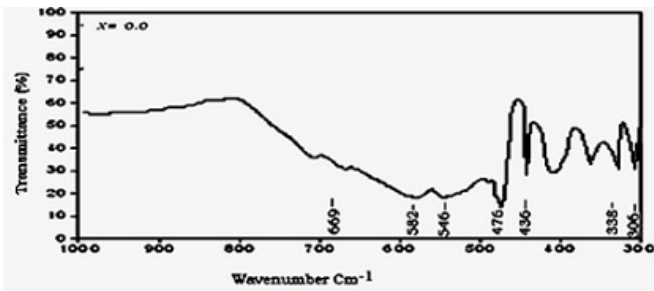


Fig.2 The IR absorption bands of $[Li_{0.5+x}Sb_xFe_{2.5-2x}]O_4$, where 'x' =0.0 concentration of antimony substitution

Table 4: Force constant (K), Elastic wave velocities (V_l & V_s), stiffness constant (C_{ij}), Young's modulus (E), rigidity modulus (n), Bulk modulus (K), mean velocity (V_m), Poisson's ratio (σ) and Debye temperature (θ_D) of $Li_{0.5}Fe_{2.5}O_4$ ferrite.

Content x	V_l (m/s)	V_s (m/s)	K (N/m^2)	n (N/m^2)	E (N/m^2)	σ	V_m (m/s)	θ_D (K)
0.0	5638.77	3255.64	8.28×10^{10}	4.97×10^{10}	12.433×10^{10}	0.25	3615.27	492

From Table 4 the calculated value of elastic moduli and Debye temperature from IR spectrum for $x=0.0$ are in good agreement with which are obtained from UPT technique (Table1).

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