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Research paper

Elastic wave speeds, Debye temperature and microhardness of YX_3 (X = In, Sn, Tl and Pb) intermetallic compounds

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Abstract

In the present work, we reviewed and report on the theoretical prediction of the longitudinal, transverse and average elastic wave velocities, and the Debye temperature for some nonmagnetic YX_3 (X = In, Sn, Tl, and Pb) intermetallic compounds with stable cubic $AuCu_3$-type structure. The lattice parameters and the elastic constants used here are taken from the work of Abraham et al [1] using the generalized gradient approximation (PBE-GGA). Our results are analyzed and compared with the available theoretical and experimental data, and in general a good agreement is found. The deviation between our value (224.4 K) of the Debye temperature θ_D for YSn_3 material and the experimental one (210 K) is around 6.62%, while the deviation between our result (1401 m/s) of the transverse elastic wave velocity for YTl_3 intermetallic material and the calculated one (1470 m/s) is about 4.93%. In addition the Young's Modulus and Poisson's Ratio of YX_3 intermetallic compounds for the crystallographic planes (100), (110) and (111) are predicted.

Keywords: *YX3 (X = In, Sn, Tl and Pb) Intermetallic Compounds; Elastic Wave Velocity; Debye Temperature; Microhardness.*

1. Introduction

The Yttrium-based rare-earth intermetallic compoundsYX_3 have been the subject of many theoretical and experimental investigations due to their extensive applications in the field of industry and technology [1-3]. Abraham et al. [1] have studied the structural, electronic, optical, elasticand thermal properties of the isostructural and isoelectronic nonmagneticYX_3 (X = In, Sn, Tl, and Pb) intermetallic compoundsusing the density functional theory (DFT). They found that the calculated elastic constants satisfy the necessary mechanical stability criterions, which indicate the stability of the four intermetallic compounds in $AuCu_3$-type structure atambient conditions.
Using the density functional theory (DFT) with the full-potential linear augmented plane wave (FP-LAPW) method, Ram et al. [2] have studied the electronic structure, Fermi surface, and elastic properties of $LaSn_3$ and YSn_3 intermetallic compounds. They found that the elastic constants increase with pressure for both compounds and satisfy the conditions for mechanical stability under pressure.
Kawashimaet al. [3] found that all YX_3 (X = In, Tl, and Pb) intermetallic compounds are superconductors with a superconducting transition temperature Tc of 0.78 K for YIn_3, 1.5 K for YTl_3, and 4.72 K for YPb_3, respectively.
Using the full-potential linear augmented plane wave (FP-LAPW) method, Ram et al. [4] have investigated the electronic structures, densities of states, Fermi surfaces and elastic properties of AB_3 (A = Y, La; B = Pb, In, Tl) intermetallic compounds under pressure, while Cao et al. [5] have studied the electron-phonon interaction and superconductivity in representative $AuCu_3$-type intermetallic compounds using first-principles density functional theory (DFT) calculations.
Many other theoretical works [6-10] have studied the masse density, the longitudinal, transverse andaverage elastic wave speeds as well as the Debye temperature of several alloys and compounds.
In the present work, we reviewed and report on themasse density, the longitudinal, transverse andaverage elastic wave velocities, the Debye temperature,Vickers microhardness andthe universal anisotropy factor for $AuCu_3$-type YX_3 (X = In, Sn, Tl, and Pb) non magnetic intermetallic compounds using the lattice constants and the elastic constants of Abraham et al. [1].

2. Theory, results and discussion

The theoretical massedensity ρof a material is related to the chemical composition and crystal structure. It is obtained by dividing the mass of the atoms existing in the unit cell on the unit cell volume V. If the mass of the atoms is given in atomic mass unity (amu), it's necessary to divide them by the Avogadro number N_A. The relationship between density and crystal structure illustrates how the crystal chemistry can sometimes be used to predict the magnitude of a physical property [11]. The formula of the theoretical masse density is given by the following expression [11]:

$$\rho = MZ/N_A V \quad (1)$$

where M is the molecular weight, Z is the number ofmolecules per unit cell, N_A is the Avogadro number ($N_A = 6.022 \times 10^{23}$ mol^{-1}), and V is the unit cell volume.
For a triclinic crystal, the unit cell volume V is given by the following expression [11]:

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma)^{1/2} \quad (2)$$

where a, b, c are the cell dimensions and α, β, γ are the interaxial.
For cubic $AuCu_3$-type structure of YX_3 (X = In, Sn, Tl, and Pb) intermetallic compounds, there is only one molecule which formed from 4 atoms per unit cell (Z = 1), so the molecular density $d_M = 1/a^3$, where a is the lattice parameter. Specifically, the atoms on the cornerare shared by eight unit cells and so are counted as 1/8 in the unit cell, and the atoms on the face is shared by two unit cells and so are counted as 1/2 in the unit cell. Hence, there are 8 x (1/8) + 6 x (1/2) atoms in cubic $AuCu_3$-type structure unit cell. So, in the previous expression, the unit cell volume $V = a^3$, where a is lattice parameter.
The Debye temperature θ_D of crystal represents the highest mode of vibration, during phonon vibrations [12], θ_D is an important thermodynamical quantity, which describe various physical properties of solid that are related to lattice vibrations [13], [14]. The Debye temperature θ_D is usually calculated from the high capacity or from the elastic constants measurement [15-17]. Within the isotropic continuum approximation, the average sound velocity v_m and the Debye temperature θ_D are related by [18]:

$$k_B\theta_D = \hbar q_D v_m \quad (3)$$

where $q_D = (6\pi n_a)^{1/3}$, and n_a is the atom concentration.
For more details on the calculation of the longitudinal v_l, transverse v_t and mean v_m acoustic wave speeds of the aggregate polycrystalline solids, plrase see for example the Refrences [19-22].
Using the lattice parameters and the elastic constants of Abraham et al [1], the values of the ρ, v_l, v_t, v_m, and θ_D for YX_3 (X = In, Sn, Tl, and Pb) materials are presented in Table 1. Meanwhile, our data are compared with the available theoretical [2, 4, 5] and experimental [3] results. We can see that YIn_3 compound has the higher θ_D, indicating that this compound is most stiffened material than other ones.

Table 1: Masse Density, Longitudinal, TransverseandAverage Elastic Wave Velocities, and Debye Temperature of YX_3(X =In, Sn, Tl, And Pb) Intermetallic Compounds in Comparison with Other Available Theoretical [2], [4], [5] and Experimental [3] Data

Material	M (10^{-3} kg/mol)	ρ (kg/m^3)	v_l (m/s)	v_t (m/s)	v_m (m/s)	θ_D(K)
YIn_3	433.366	7166	3692,3750 [4]	2100,2000 [4]	2334	237.4, 234.9 [4], 217 [5]
YSn_3	445.036	7032	3714,3590 [2]	2008,1630 [2]	2241	224.4, 188.4 [2], 210 [3], 172 [5]
YTl_3	702.046	10708	2690,2920 [4]	1401,1470 [4]	1568	155.2, 168.7 [4], 139 [5]
YPb_3	710.506	10121	2657,2750 [4]	1176,1160 [4]	1327	128.4, 129.8 [4], 101 [5]

For YSn_3 material, the deviation on the longitudinal elastic wave velocityv_l between our result (3714 m/s) and that (3590 m/s) of Ram et al. [2] is only about 3.34%, and a good agreement is obtained. The deviation between our value (224.4 K) of the Debye temperature θ_D for YSn_3 intermetallic material and the experimental one (210 K) [3] is around 6.62%.
For monocrystalin material, the Young's modulus and the Poisson's ratio are related to the crystallographic directions [23]. The Young's modulus and the Poisson's ratio within the crystallographic planes (100), (110) and (111) for YX_3 (X = In, Sn, Tl, and Pb) intermetallic compounds have be calculated using the expressions reported in Ref. [23] and in Table 3.13 (page 54) of Ref. [24]. The shame expressions are successfully applied for K_2TlAsX_6 (X = Cl, Br) semiconducting materials [23]. The obtained values of the Young's modulus and the Poisson's ratio for YX_3 (X = In, Sn, Tl, and Pb) materials are tabulated in Table 2.

Table 2: Young's Modulus and Poisson's Ratio within the Crystallographic Planes (100), (110) and (111) for YX_3(X =In, Sn, Tl, and Pb) Intermetallic Compounds, m Is the Direction for A Longitudinal Stress, While n Is the Direction for A Transverse Strain (Orthogonal to the Direction m)

Parameter	Plane	Direction	YIn_3	YSn_3	YTl_3	YPb_3
Young's modulus (GPa)	(100) plane	[001] direction	93.71	54.81	63.97	16.46
		[011] direction	75.84	76.71	52.86	37.46
	(110) plane	[001] direction	93.71	54.81	63.97	16.46
		[111] direction	71.30	88.49	49.97	65.18
	(111) plane		75.84	76.71	52.86	37.46
Poisson's ratio	(100) plane	m = [010], n = [001]	0.22	0.35	0.28	0.45
		m = [011], n = [$0\bar{1}1$]	0.37	0.08	0.41	- 0.26
	(110) plane	m = [001], n = [$1\bar{1}0$]	0.22	0.35	0.28	0.45
		m = [$1\bar{1}1$], n = [$1\bar{1}\bar{2}$]	0.29	0.25	0.33	0.29
	(111) plane		0.24	0.35	0.29	0.59

From the previous table, we can see for YIn_3 compound that the maximum value E_{max} of Young's modulus was obtained at around 93.71 GPa within (110) crystallographic plane and in [001] direction, while the minimum value E_{min} was obtained at around 71.3 GPa within (100) plane and in [111] crystallographic direction, which gives a ratio of $E_{max}/E_{min} \approx 1.31$.
There are different relationships frequently employed to predict the hardness H of the materials [25-30]. We calculate the Vickers microhardness H_V of YX_3 (X = In, Sn, Tl, and Pb) materials using the following expression [31, 32]:

$$H_V = 0.92(G/B)^{1.137}G^{0.708} \quad (4)$$

where G is the shear modulus and B is the bulk modulus.
Our calculated values of the Vickers hardness H_V are 5.58 GPa for YIn_3, 4.25 GPa for YSn_3, 3 GPa for YTl_3 and 1.32 GPa for YPb_3 intermetallic compound, respectively. To the best of author knowledge, there is no any data in the literature on the Vickers microhardness-for YX_3 (X = In, Sn, Tl, and Pb) intermetallic compounds to make comparaison.

To provide an accurate measure of anisotropy, the Zener anisotropy factor A was frequently used in cubic crystals [33], [34]. The universal anisotropy factor (A^U) was often used to all the crystal symmetries, it is referred to as universal anisotropy factor; it can be written as: $A^U = 5(G_V/G_R) + (B_V/B_R) - 6 \geq 0$ [35-37]. For isotropic material, A^U is zero [35]. The non-zero values: ~ 0.13 for YIn_3, ~ 0.38 for YSn_3, ~ 0.10 for YTl_3 and ~ 3.19 for YPb_3, respectively of A^U indicate the anisotropic nature of YX_3 (X = In, Sn, Tl, and Pb) compounds, which becomes higher for YPb_3 intermetallic compound. These results are in accord with the results of Aobtained by Abraham et al. [1].

3. Conclusion

In conclusion, we reviewed and report on the longitudinal, transverse andaverage elastic wave velocities, and Debye temperature of YX_3 (X = In, Sn, Tl, and Pb) intermetallic compounds using the lattice parameters and the elastic constants obtained by Abraham et al.[1]. Our results are analyzed and compared with the available theoreticaland experimental data, and in general a good agreement is found. The deviation between our value (224.4 K) of θ_D for YSn_3 material and the experimental one (210 K) is around 6.62%. In addition, we calculate the Vickers microhardness H_V of YX_3 (X = In, Sn, Tl, and Pb) intermetallic compounds, which are 5.58 GPa for YIn_3, 4.25 GPa for YSn_3, 3 GPa for YTl_3, and 1.32 GPa for YPb_3 compound, respectively. These results of the microhardness are in accord with the results of the Debye temperature, thus because in general, there is correlation between these two quantities.

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