ISSN : 0974 - 7494 Volume 7 Issue 6

Nano Science and Nano Technology
An Indian Journal

Full Paper

NSNTAIJ, 7(6), 2013 [205-208]

Elastic and acoustic properties of intermetallic nanostructure $SrGa_2$ compound

Pramod Kumar Yadawa
Department of Applied Physics, AMITY School of Engineering and Technology,
Bijwasan, New Delhi-110 061, (INDIA)
E-mail : pkyadawa@rediffmail.com

ABSTRACT

The ultrasonic properties like ultrasonic sound velocity in the hexagonal structured intermetallic nanostructure $SrGa_2$ compound has been studied along unique axis at room temperature. The second- and third order elastic constants (SOEC & TOEC) have been calculated for this compound using Lennard–Jones potential. The velocity V_L and V_{S2} increases with the angle from unique axis, while V_{S1} and V_D have maxima with 45^0 with unique axis of the crystal. The inconsistent behaviour of angle dependent velocities is associated to the action of second order elastic constants. Debye average sound velocities of $SrGa_2$ are increasing with the angle and has maximum at 45^0 with unique axis at room temperature. Hence when a sound wave travels at 45^0 with unique axis of $SrGa_2$ compound, then the average sound velocity is found to be maximum. The mechanical properties of $SrGa_2$ are better than other intermetallic compounds $BaGa_2$ and $CaGa_2$ at room temperature, because it has high ultrasonic velocity and low ultrasonic attenuation. The comparison of calculated ultrasonic parameters with available theoretical/experimental physical parameters gives information about classification of this compound.

KEYWORDS

Intermetallic nanostructure compound;
Elastic properties;
Ultrasonic properties.

INTRODUCTION

Ultrasonic offer the possibility to detect and characterize microstructral properties as well as flaws in nanomaterials, controlling materials behaviour based on physical mechanism to predict future performance of the nanomaterials. Various investigators have shown considerable interest on ultrasonic properties of different materials. Wave propagation velocity is key parameter in ultrasonic characterization and can provide information about crystallographic texture. The ultrasonic velocity is directly related to the elastic constants by the relationship $V=\sqrt{(C/\rho)}$, where C is the relevant elastic constants and ρ is the density of that particular material. Also ultrasonic attenuation is very important physical parameter to characterize the material, which is well related to several physical quantities like thermal conductivity, specific heat, thermal energy density and higher order elastic constants[1,2]. The elastic constants provide valuable information about the bonding characteristic between adjacent atomic planes and the anisotropic character of the bonding and structural stability[3,4].

Full Paper

Acoustic phonon dispersion curves have been determined by inelastic neutron scattering in the intermetallic nanostructure compound $SrGa_2$. The intermetallic compound $SrGa_2$ has a hexagonal structure[5]. The electronic structure and chemical bonding are experimentally calculated by F.Haarmann et.al[6]. There are three types of acoustic mode lattice vibration: one longitudinal acoustic and two transverse acoustical for hexagonal and cubic structured materials[7,8]. Hence, there are three types of acoustic wave velocities for each direction of propagation of wave, which are well related to second order elastic constants. But elastic constants of $SrGa_2$ and all the three type of orientation dependent acoustic wave velocity of this compound is not reported in literature.

Therefore, in this work we predict the ultrasonic properties of hexagonal structured $SrGa_2$ at room temperature. The higher order elastic constants and ultrasonic wave velocities for $SrGa_2$ for each direction of propagation of wave are calculated at room temperature. The calculated ultrasonic parameters are discussed with related thermophysical properties for the characterization of the chosen materials. The obtained results are analyzed in comparison to other hexagonal structured materials.

THEORY

In the present investigation, the theory is divided into two parts:

Second and third order elastic cnstants

The second (C_{IJ}) and third (C_{IJK}) order elastic constants of material are defined by following expressions.

$$C_{IJ} = \frac{\partial^2 U}{\partial e_I \partial e_J}; \qquad I \text{ or } J = 1,.....6 \tag{1}$$

$$C_{IJK} = \frac{\partial^3 U}{\partial e_I \partial e_J \partial e_K}; \; I \text{ or } J \text{ or } K = 1,.....6 \tag{2}$$

where, U is elastic energy density, $e_I = e_{ij}$ (i or j = x, y, z, I=1, …6) is component of strain tensor. Equations (1) and (2) leads six second and ten third order elastic constants (SOEC and TOEC) for the hexagonal close packed structure materials[1,9].

$$\left.\begin{array}{ll} C_{11} = 24.1\,p^4C' & C_{12} = 5.918\,p^4C' \\ C_{13} = 1.925\,p^6C' & C_{33} = 3.464\,p^8C' \\ C_{44} = 2.309p^4C' & C_{66} = 9.851\,p^4C' \end{array}\right\} \tag{3a}$$

$$\left.\begin{array}{ll} C_{111} = 126.9p^2B + 8.853p^4C' & C_{112} = 19.168p^2B - 1.61p^4C' \\ C_{113} = 1.924p^4B + 1.155p^6C' & C_{123} = 1.617p^4B - 1.155p^6C' \\ C_{133} = 3.695p^6B & C_{155} = 1.539p^4B \\ C_{144} = 2.309p^4B & C_{344} = 3.464p^6B \\ C_{222} = 101.039p^2B + 9.007p^4C' & C_{333} = 5.196p^8B \end{array}\right\} \tag{3b}$$

where p = c/a: axial ratio; $C' = \chi\, a / p^5$; $B = \psi\, a^3 / p^3$;

$\chi = (1/8)[\{nb_0\,(n-m)\}/\{a^{n+4}\}]$ $\psi = -\chi/\{6\,a^2(m+n+6)\}$;

m, n=integer quantity; b_0=Lennard Jones parameter.

Acoustic wave velocity in hexagonal structured crystal

The anisotropic behaviour of the material can be understood with the knowledge of ultrasonic velocity because the velocity is related to the second order elastic constants[10]. On the basis of mode of atomic vibration, there are three types of velocities (longitudinal, quasi shear and shear) in acoustical region[11]. These velocities vary with the direction of propagation of wave from the unique axis of hexagonal structured crystal[12]. The ultrasonic velocities as a function of angle between direction of propagation and unique axis for hexagonal structured materials are[13]:

$$V_L^2 = \{C_{33}Cos^2\theta + C_{11}Sin^2\theta + C_{44} + \{[C_{11}Sin^2\theta - C_{33}Cos^2\theta + C_{44}(Cos^2\theta - Sin^2\theta)]^2 + 4\,Cos^2\theta\,Sin^2\theta\,(C_{13}+C_{44})^2\}^{1/2}\}/2\rho \tag{4}$$

$$V_{S1}^2 = \{C_{33}Cos^2\theta + C_{11}Sin^2\theta + C_{44} - \{[C_{11}Sin^2\theta - C_{33}Cos^2\theta + C_{44}(Cos^2\theta - Sin^2\theta)]^2 + 4\,Cos^2\theta\,Sin^2\theta\,(C_{13}+C_{44})^2\}^{1/2}\}/2\rho \tag{5}$$

$$V_{S2}^2 = \{C_{44}Cos^2\theta + C_{66}Sin^2\theta\}/\rho \tag{6}$$

where V_L, V_{S1} and V_{S2} are longitudinal, quasi shear and pure shear wave ultrasonic velocities. Variables ρ and q represent the density of the material and angle with the unique axis of the crystal respectively. The Debye temperature (T_D) is an important physical parameter for the characterization of materials, which is well related to the Debye average velocity (V_D).

$$T_D = \frac{\hbar\, V_D\,(6\pi^2\, n_a)^{1/3}}{K_B} \tag{7}$$

$$\text{here } V_D = \left\{ \frac{1}{3}\left(\frac{1}{V_L^3} + \frac{1}{V_{S1}^3} + \frac{1}{V_{S2}^3} \right) \right\}^{-1/3} \quad (8)$$

where $\hbar$ is quantum of action and is equal to Planck's constant divided by 2π; K_B is Boltzmann Constant; n_a is atom concentration.

RESULTS AND DISCUSSION

Higher order elastic constants

The unit cell parameters 'a' (basal plane parameter) and 'p' (axial ratio) for $SrGa_2$ are 4.34Å and 1.089 respectively[5,6]. The value of m and n for chosen nanomaterials are 6 and 7. The value of b_0 is 2.2×10^{-65} erg cm^7 for $SrGa_2$. The SOEC and TOEC have been calculated for $SrGa_2$ using equation. (3) and are presented in TABLE 1.

The elastic constants are important since they are related to hardness and are used for the determination of the ultrasonic velocity. It is obvious from TABLE 1 that, there is good agreement between the present and reported theoretical/experimental second order elastic constants of $SrGa_2$[5]. Thus our theoretical approach for the calculation of second order elastic constants for hexagonal structured intermetallic nanostructure compound at room temperature is well justified. However, third order elastic constants are not compared due to lack of data in the literature but the negative third order elastic constants are found in previous papers for hexagonal structure materials[14,15]. Hence applied theory for the evaluation of higher order elastic constants at room temperature is justified. The bulk modulus (B) for this material can be calculated with the formula $B = 2(C_{11} + C_{12} + 2C_{13} + C_{33}/2)/9$. The evaluated B for this intermetallic nanomaterial is presented in TABLE 1.

Ultrasonic velocity and allied parameters

The computed orientation dependent ultrasonic wave velocities and Debye average velocities at 300 K are shown in Figures 1–2. Figures 1–2 show that the The velocity V_L and V_{S2} increases with the angle from unique axis, while V_{S1} and V_D have maxima with 45^0 with unique axis of the crystal. The inconsistent behaviour of angle dependent velocities is associated to the action of second order elastic constants. The combined effect of SOEC and density is reason for abnormal behaviour of angle dependent velocities.

TABLE 1 : Second and third order elastic constants (SOEC and TOEC) & bulk modulus (B) in the unit of 10^{10} Nm^{-2} of $SrGa_2$ at room temperature.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B
$SrGa_2$	12.78	4.14	1.21	7.58	1.453	5.014	2.35
Ref[5]	12.62	5.14		7.29	2.81	3.76	

	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{344}	C_{144}	C_{155}	C_{222}	C_{333}
$SrGa_2$	-208.51	-33.06	-3.11	-3.95	-8.73	-8.19	-4.60	-3.07	-164.98	-14.56

The nature of the angle dependent velocity curves in the present work is found similar as that for hexagonal structured titanium diborieds and other nanostructure materials. The chosen nanomaterial has shown similar properties with their crystal structure. Thus the angle dependency of the velocities in this intermetallic compound is justified.

Since ultrasonic attenuation (A) is directly correlated with velocity (V) as $A \propto V^{-3}$[16] and velocity of $SrGa_2$ is larger than other intermetallic compounds $BaGa_2$ and $CaGa_2$[6], thus the attenuation of $SrGa_2$ should be smallest and material should be most ductile. The minimum ultrasonic attenuation justifies its quite stable hexagonal structure state. Also $SrGa_2$ has maxi-

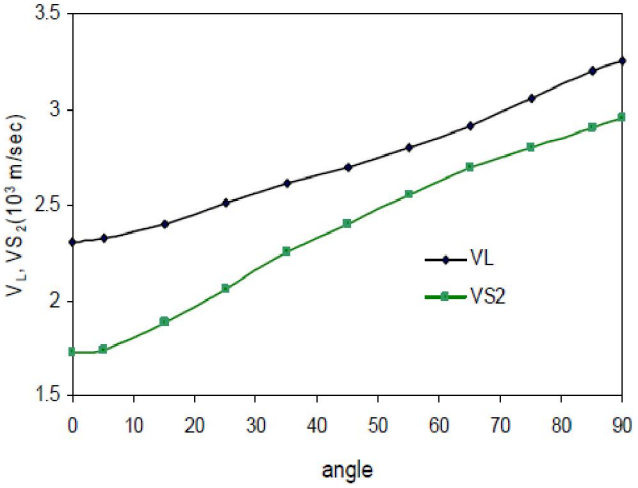

Figure 1 : V_L and V_{S2} vs angle with unique axis of crystal

Full Paper

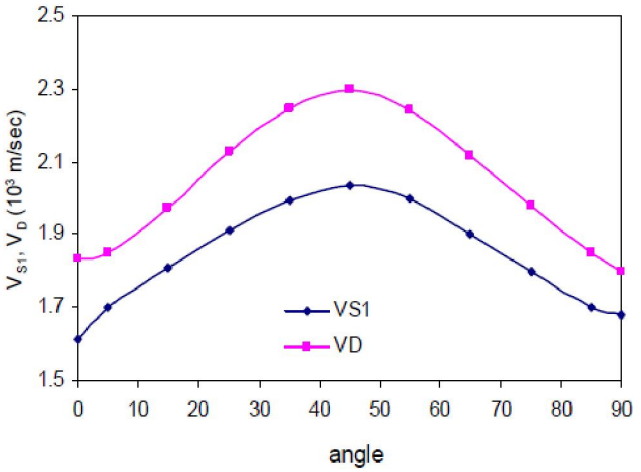

Figure 2 : V_{S1}, V_D vs angle with unique axis of crystal

mum elastic constants and bulk modulus among others. Hence $SrGa_2$ is more ductile, stable and contain few defects in the crystal structure in comparison to other intermetallic compounds.

CONCLUSIONS

On the basis of above discussion, we conclude following points:

- Our theory of higher order elastic constants is justified for the hexagonal structured intermetallic nanomaterials.
- All elastic constants are mainly the affecting factor for anomalous behaviour of acoustical velocity in reported intermetallic compound.
- The average sound velocity is a direct conse quence of Debye temperature, specific heat and thermal energy density of these compounds.
- The mechanical properties (yield strength, ductility, elastic properties etc.) of $SrGa_2$ are better than other intermetallic compounds $BaGa_2$ and $CaGa_2$ at room temperature, because it has high ultrasonic velocity and low ultrasonic attenuation.

Thus obtained results in the present work can be used for further investigations, general and industrial applications. Our theoretical approach is valid for ultrasonic characterization of these compounds at room temperature. The acoustic behavior in these nanomaterials as discussed above shows important microstructural characteristic feature, which are well connected to thermoelectric properties of the materials.

ACKNOWLEDGMENTS

The author wish to express sincere thanks to Dr. Ashok K. Chauhan, President, AMITY School of Engineering and Technology (ASET), New Delhi, Prof. B. P. Singh, Senior Director, Prof. (Dr.) Rekha Agarwal, Director, ASET New Delhi, Prof. S. K. Kor and Prof. Raja Ram Yadav, Department of Physics, Allahabad University, for encouraging and providing necessary facilities in carrying out the work.

REFERENCES

[1] P.K.Yadawa, D.Singh, D.K.Pandey, R.R.Yadav; The Open Acoustic Journal, **2**, 80 **(2009)**.
[2] D.Singh, P.K.Yadawa; Platinum Metals Rev., **54(3)**, 172 **(2010)**.
[3] P.Ravindran, L.Fast, P.A.Korzhavyi, B.Johansson, J.M.Wills, O.Eriksson; J.Appl.Phys., **84**, 4891 **(1998)**.
[4] F.Hong-Zhi, L.D-Hua, P.Feng, G.Tao, C.Xin-Lu; Commun.Theor.Phys., **50**, 1427 **(2008)**.
[5] H.Meyer, A.Weiss, B.Dorner; Solid State Communication, **25**, 1093 **(1978)**.
[6] F.Haarmann, K.Kach, D.Griner, W.Schnelle, O.Pecter, R.Cardoso-Gil, H.Borrmann, H.Rosner, Y.Grin; **15**, 1673 **(2009)**.
[7] M.Rosen, H.Klimker; Phys.Rev.B., **1(9)**, 3748 **(1970)**.
[8] G.A.Alers, J.R.Neighbours; J.Phys.Chem.Solids, **7**, 58 **(1958)**.
[9] A.K.Yadav, R.R.Yadav, D.K.Pandey, D.Singh; Mat.Lett., **62**, 3258 **(2008)**.
[10] C.Oligschleger, R.O.Jones, S.M.Reimann, H.R.Schober; Phys.Rev.B, **53**, 6165 **(1996)**.
[11] D.K.Pandey, D.Singh, R.R.Yadav; Appl.Acoust., **68**, 766 **(2007)**.
[12] D.K.Pandey, P.K.Yadawa, R.R.Yadav; Mat.Lett., **61**, 4747 **(2007)**.
[13] D.K.Pandey, P.K.Yadawa, R.R.Yadav; Mat.Lett., **61**, 5194 **(2007)**.
[14] D.K.Pandey, D.Singh, P.K.Yadawa; Plat.Met.Rev., **53**, 91 **(2009)**.
[15] P.K.Yadawa; The Arabian Journal for Science and Engineering, **37**, 225 **(2012)**.
[16] P.K.Yadawa; Ceramics-Silikaty, **55**, 127 **(2011)**.