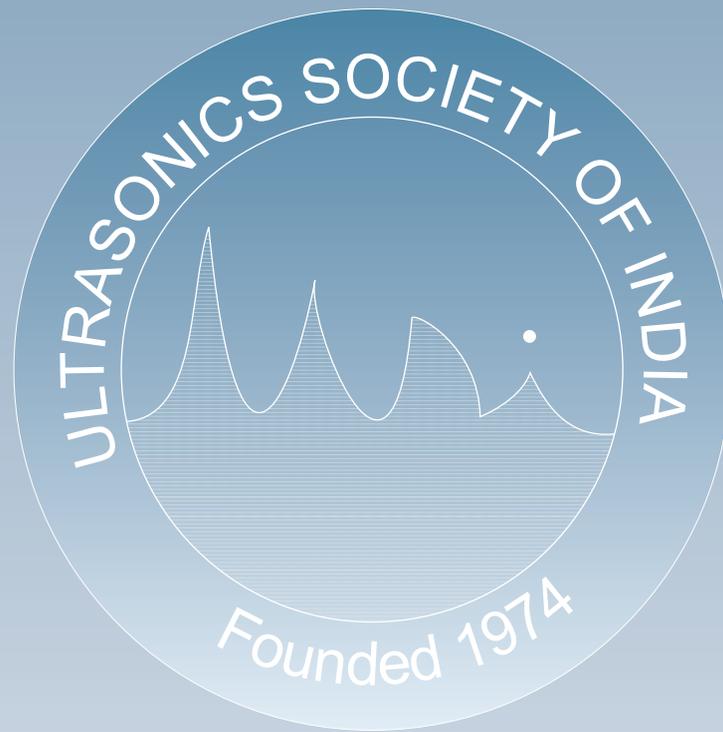


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CONTENTS

Ultrasonic studies on binary mixtures of 1,4-dichlorobutane with some hydrocarbons at 308.15K, 313.15K and 318.15K Kanchan Yadav and S. S. Yadava	1
Study of physical and acoustical properties of nuclear extractant Abhijit Sarangi, Ranjeeta Giri, Ganeswar Nath and Rita Paikaray	8
Ultrasonic investigations of molecular interaction in binary mixtures of ellagic acid with acetone G.M. Jamankar and M.S. Deshpande	12
Elastic and acoustic properties of hexagonal intermetallic ternary compound Pramod Kumar Yadawa	16
A simple sonication-assisted exfoliation and characterization of few layered graphene nanosheets Rintu Varghese, H. Joy Prabu and I. Johnson	22
NDT 2018: Call for Papers	25
PhD Thesis Summary	26
National Symposium on Advances in Ultrasonics and Materials Research	27
An Obituary — Dr. Baldev Raj	30

(Authors have stated that the papers have not been published elsewhere)

Ultrasonic studies on binary mixtures of 1,4-dichlorobutane with some hydrocarbons at 308.15K, 313.15K and 318.15K

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Ultrasound velocity and density of the binary mixtures of 1, 4-dichlorobutane with several hydrocarbons such as cyclohexane, benzene, methylbenzene, 1, 2-dimethylbenzene, 1, 4-dimethylbenzene and 1,3,5-trimethylbenzene have been measured over entire mole fractions range at three temperatures 308.15K, 313.15K, and 318.15K. Adiabatic compressibility has been evaluated from the experimental data. Ultrasound velocities increase with mole fractions of 1, 4-dichlorobutane at all the three experimental temperatures for 1, 4-dichlorobutane + cyclohexane system. The ultrasonic velocity decreases with molefractions of 1, 4-dichlorobutane for binary mixtures with all the aromatic hydrocarbons used at the three experimental temperatures. The adiabatic compressibilities decrease with mole fractions of 1, 4-dichlorobutane for all the binary mixtures studied at the three experimental temperatures. The deviations in adiabatic compressibilities from the ideal values have also been evaluated. At higher temperature, the values of ultrasonic velocity decreases while adiabatic compressibility increases for all the binary mixtures. The results are interpreted in terms of molecular interactions operating between the components of the binary mixtures.

Keywords: Ultrasound velocity, binary mixtures, 1,4-dichlorobutane, aromatic hydrocarbons.

Introduction

The measurement of ultrasound velocity, density, and evaluation of several other acoustical parameters for binary liquid mixtures have attracted the attention of several investigators¹. Physical properties of the liquid mixtures containing non-electrolyte liquid as components give information about the interactions between the components and about the structure of the liquid mixtures. Speeds of sound have been measured and isentropic compressibilities have been determined for binary mixtures of methyl and pentyl ethanoate with di-, tri-, and tetrachloroethane² and the analysis of the data has been made on the basis of molecular interactions. Ultrasonic studies have also been made for binary mixtures where one component is tetrachloroethylene and tetrachloroethane³.

Benzene and dimethylbenzene are used as diluent⁴ for extractant, acetylacetone which is used in extraction

process of various metals. It has been suggested that 1, 4-dichlorobutane either alone or with other scavenging materials in admixture with lead antiknock compounds in fuels is always effective scavenger⁵ and is equally good as those in commercial use. In view of the above 1, 4-dichlorobutane has been chosen as one component of the binary mixtures in the present investigation. The second components are aromatic hydrocarbons such as benzene, methyl benzene, 1, 2-dimethyl benzene, 1, 4-dimethyl benzene and 1, 3, 5-trimethyl benzene. These are chosen keeping in mind that the study will provide information about the behaviour of liquid mixtures on changing benzene with either methylated benzene or dimethylated benzenes. The binary mixture of 1, 4-dichlorobutane with cyclohexane having six membered ring as that of aromatic hydrocarbons used in this investigation but without π -electrons has also been investigated in order to have a reference point for comparison of molecular interactions.

Materials and Methods

Chemicals used were cyclohexane (98.7%), benzene (99.7%), methyl benzene (99.96%), 1, 2-dimethyl benzene ($\geq 98\%$), 1,4-dimethyl benzene ($\geq 99\%$), 1,3,5-trimethyl benzene ($\geq 98\%$) and 1,4-dichlorobutane (98%). These chemicals were further purified by distilling over different size columns (*viz.* for cyclohexane and benzene 100 cm long column, for methylbenzene 60 cm long column and for remaining others 30 cm long column) and only middle fractions were collected and used for binary sample preparation. Purities of the distilled chemicals were checked by comparing experimental values of densities with those of literature values and a good agreement was found between the two.

Binary liquid mixtures of 1, 4-dichlorobutane with hydrocarbon solvents were prepared gravimetrically covering whole molefraction range. The component liquids were injected into glass sealed vials employing syringes with 24 number needle to avoid evaporation losses during sample preparation. All the masses were measured within $\pm 1 \times 10^{-8}$ kg by using single pan analytical balance.

Ultrasound velocities of the different samples were measured by M-82 multifrequency ultrasonic interferometer at a constant frequency of 2 MHz and at three constant experimental temperatures. The minimum amount of liquid needed was about 0.01 L. The samples were placed in the cell having micrometer with least count $\pm 1.0 \times 10^{-5}$ m. The temperature of the cell was maintained constant at experimental temperatures 308.15 K, 313.15 K, and 318.15 K within ± 0.03 K by circulating thermostated water around the interferometer cell by means of circulating pump. The micrometer was moved upward and the distance, '*d*', moved by micrometer for 20 maxima on current meter of the interferometer was recorded. The '*d*' is related with the wavelength, λ of the ultrasonic wave as follows :

$$d = n.\lambda/2 \quad (1)$$

Here $n=20$. The ultrasonic velocity, was determined by Eq. (2),

$$u = v.\lambda \quad (2)$$

where v is the frequency of the quartz crystal generating ultrasound waves. Triplicate measurements for each sample were taken and the average value for ultrasound velocity was taken accurate to $\pm 0.03\%$. Densities of the

pure samples and their mixtures were measured at experimental temperatures employing single stem pyknometer and recorded after making buoyancy correction⁶. The uncertainty in density measurement was determined by GUM type A method⁷ and was found to be $\pm 0.05 \text{ kg.m}^{-3}$.

Experimental values of ultrasound velocities, '*u*' and densities, ' ρ ' are used to evaluate adiabatic compressibility, β_{ad} employing Eq. (3),

$$\beta_{ad} = u^{-2}.\rho^{-1} \quad (3)$$

where β_{ad} is defined as decrease in volume caused by sudden increase of pressure per unit volume at constant entropy *i.e.*,

$$\beta_{ad} = -(1/V)(\delta V/\delta P)_s \quad (4)$$

where $-(\delta V/\delta P)_s$ is the decrease in volume with sudden increase of pressure at constant entropy and V is the molar volume.

Results and Discussion

The experimental values of ultrasound velocities, '*u*' and densities, ' ρ ' as a function of mole fractions, x_1 of 1, 4-dichlorobutane at the three experimental temperatures 308.15K, 313.15K, and 318.15K for binary mixtures of 1, 4-dichlorobutane with six hydrocarbon solvents *viz.* cyclohexane, benzene, methylbenzene, 1, 2-dimethylbenzene, 1, 4-dimethylbenzene and 1, 3, 5 -trimethylbenzene are shown in Figs.1-6.

It is evident from Figs. 1-3 that ultrasound velocities increase for binary mixtures of 1, 4-dichlorobutane + cyclohexane as molefractions (x_1) of 1, 4-dichlorobutane increase in the binary mixtures. Unlike this, when binary mixtures are prepared replacing cyclohexane with several aromatic hydrocarbons, ultrasound velocities decrease with mole fractions of 1, 4-dichlorobutane at all the three temperatures. Perusal of Figs. 1-3 also reveals that for a fixed composition of binary mixtures, ultrasound velocity decreases with increase of temperature for all the binary mixtures studied. From Figs. 1-3, it is also evident that ultrasound velocities for binary mixtures of 1, 4-dichlorobutane with benzene and with methylbenzene are quite close with each other at 308.15 K and 318.15 K. Similar behaviour is also shown by binary mixtures of 1, 4-dichlorobutane + 1, 4-dimethylbenzene and + 1, 3, 5-trimethylbenzene at 308.15 K. However, the '*u*' values at 313.15K for the binary mixture with

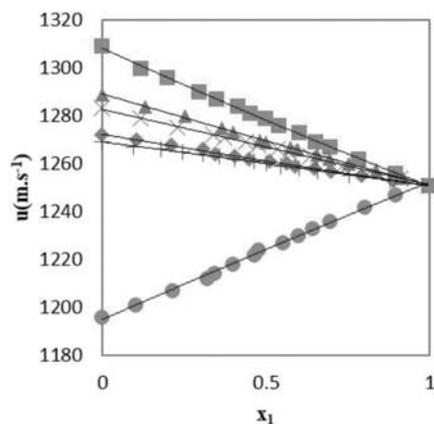


Fig. 1 Variations of ultrasound velocities (u) with mole fractions (x_1) of 1,4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2- dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 308.15K.

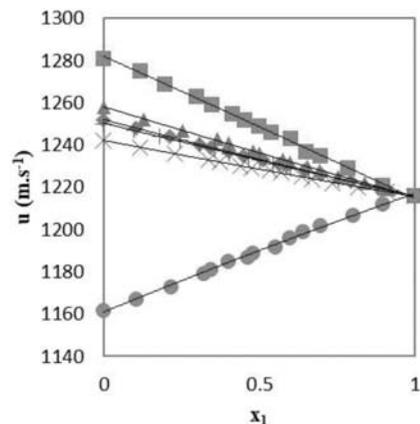


Fig. 3 Variations of ultrasound velocities (u) with mole fractions (x_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2- dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 318.15K.

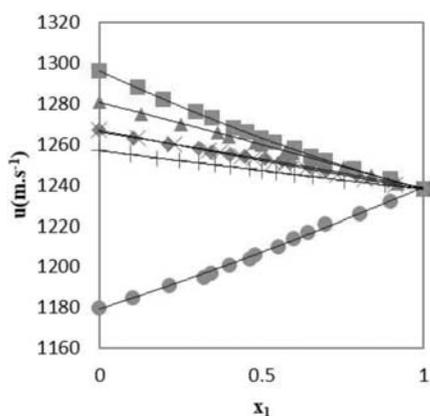


Fig. 2 Variations of ultrasound velocities (u) with mole fractions (x_1) of 1,4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2- dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 313.15K.

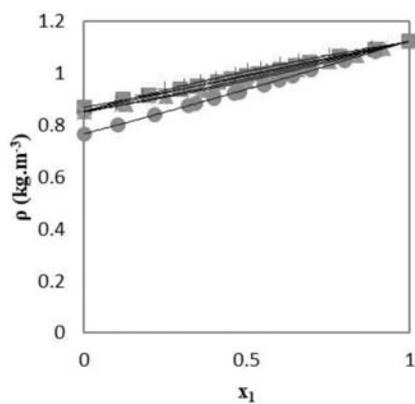


Fig. 4 Variations of densities (ρ) with mole fractions (x_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2- dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 308.15K.

methylbenzene and 1, 4-dimethylbenzene are very close to each other.

Adiabatic compressibility, β_{ad} has been evaluated by Eq. (3) and its variations with molefractions (x_1) of 1, 4-dichlorobutane for all the six binary mixtures at three temperatures have been given in Figs. 7-9.

Observations of Figs. 7-9 reveal that β_{ad} values decrease with increase in mole fractions of 1, 4-dichlorobutane in all the six binary mixtures at the

experimental temperatures. It is also evident from Figs. 7-9 that at any fixed composition of the binary mixtures, the values of β_{ad} is largest for the mixture with cyclohexane at the three experimental temperatures. However, the β_{ad} values for the binary mixtures with five aromatic hydrocarbons at the three experimental temperatures are very close with each other at any common composition for the mixtures. Adiabatic compressibility of a liquid may be measured with considerable precision and therefore, is a powerful tool

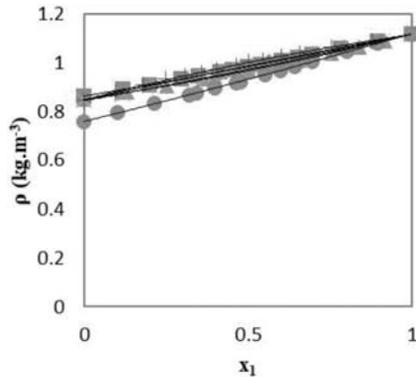


Fig. 5 Variations of densities (ρ) with mole fractions (x_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2- dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 313.15K.

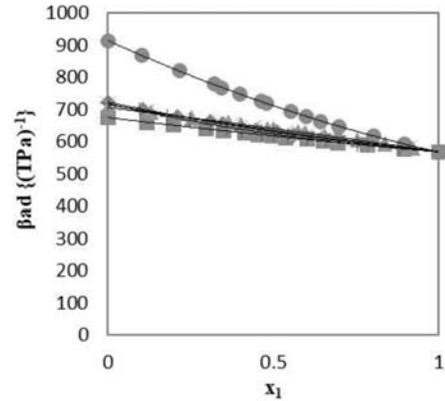


Fig. 7 Variations of adiabatic compressibilities (β_{ad}) with mole fractions (x_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1,2- dimethylbenzene (■), + 1,4-dimethylbenzene (×) and + 1,3,5-trimethylbenzene (▲) at temperature 308.15K.

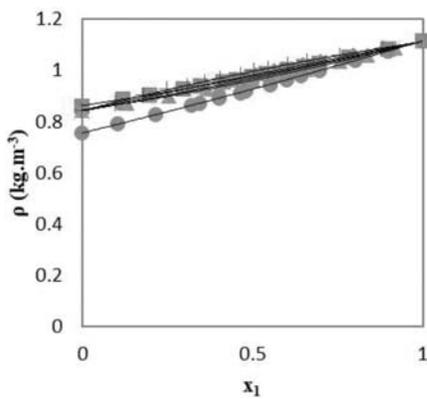


Fig. 6 Variations of densities (ρ) with mole fractions (x_1) of 1,4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2- dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 318.15K.

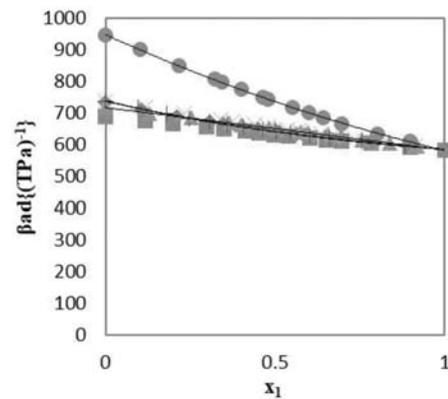


Fig. 8 Variations of adiabatic compressibilities (β_{ad}) with mole fractions (x_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (●), + benzene (+), + methylbenzene (◆), + 1, 2-dimethylbenzene (■), + 1, 4-dimethylbenzene (×) and + 1, 3, 5-trimethylbenzene (▲) at temperature 313.15 K.

for the study of deviations from ideal behavior in liquids. It has been mentioned by Jain *et al.*⁸ that excess compressibility is sensitive to any perturbation of liquid structure, and hence changes in molecular shape and the interaction potential affects its value. It is therefore a more sensitive measure of specific molecular interaction than the excess enthalpy and free energy. Keeping the above fact in mind, deviation in adiabatic compressibility β_{ad} for all binary mixtures at the three experimental temperatures are evaluated as follows :

$$\Delta\beta_{ad} = \beta_{ad} - (\phi_1\beta_{ad,1} + \phi_2\beta_{ad,2}) \quad (5)$$

where β_{ad} is the adiabatic compressibility for the binary mixtures obtained by Eq. (3) using experimental values of ultrasound velocities and densities for the mixtures. $\beta_{ad,1}$, $\beta_{ad,2}$ and ϕ_1 , ϕ_2 are the adiabatic compressibilities and the volume fractions of the components of the mixtures. The values of $\Delta\beta_{ad}$ for all the binary mixtures studied as a functions of volume fractions (ϕ_1) of 1, 4-dichlorobutane at temperatures 308.15 K, 313.15 K and 318.15 K have been shown in Figs. 10-12.

The values of $\Delta\beta_{ad}$ obtained by Eq. (5) are fitted into Redlich - Kister polynomial equation (6)

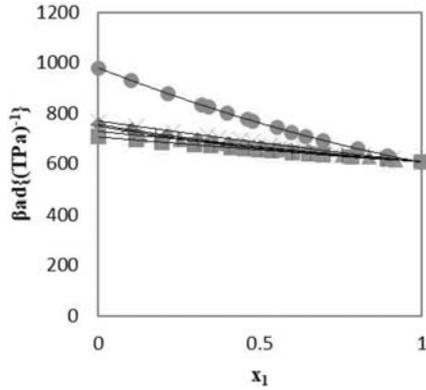


Fig. 9 Variations of adiabatic compressibilities (β_{ad}) with mole fractions (x_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (\bullet), + benzene (+), + methylbenzene (\blacklozenge), + 1, 2- dimethylbenzene (\blacksquare), + 1, 4-dimethylbenzene (\times) and + 1, 3, 5-trimethylbenzene (\blacktriangle) at temperature 318.15K.

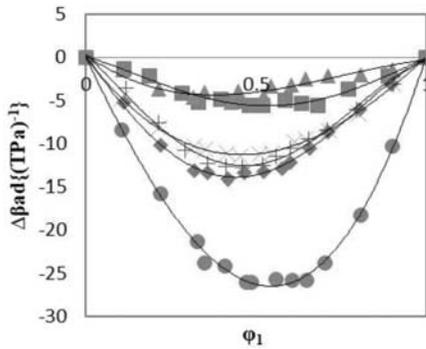


Fig. 10 Deviations in adiabatic compressibilities ($\Delta\beta_{ad}$) with volume fractions (ϕ_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (\bullet), + benzene (+), + methylbenzene (\blacklozenge), + 1, 2-dimethylbenzene (\blacksquare), + 1, 4-dimethylbenzene (\times) and + 1, 3, 5-trimethylbenzene (\blacktriangle) at temperature 308.15K. The points represent experimental values calculated from Eq. (5) and line represent R - K values calculated from Eq. (6).

$$\Delta\beta_{ad} = \phi_1(1 - \phi_1) \sum a_i(1 - 2\phi_1)^i \quad (6)$$

where a_i (a_0, a_1, a_2, \dots) are the coefficients of the polynomial. The values of the coefficients are determined by least squares method and given in Table 1. The standard deviations in deviation in adiabatic compressibility $\sigma(\Delta\beta_{ad})$ are evaluated using equation

$$\sigma(\Delta\beta_{ad}) = \left[\frac{\sum (\Delta\beta_{ad,eq(5)} - \Delta\beta_{ad,eq(6)})^2}{(n - m)} \right]^{1/2} \quad (7)$$

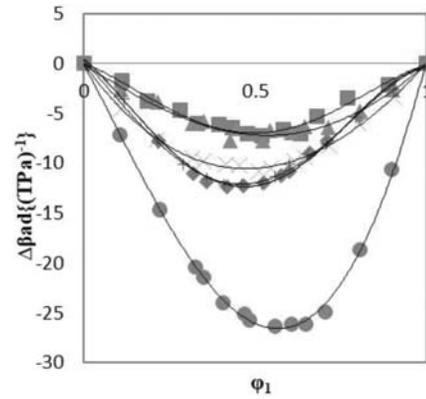


Fig. 11 Deviations in adiabatic compressibilities ($\Delta\beta_{ad}$) with volume fractions (ϕ_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (\bullet), + benzene (+), + methylbenzene (\blacklozenge), + 1, 2-dimethylbenzene (\blacksquare), + 1, 4-dimethylbenzene (\times) and + 1, 3, 5-trimethylbenzene (\blacktriangle) at temperature 313.15 K. The points represent experimental values calculated from Eq. (5) and line represent R - K values calculated from Eq. (6).

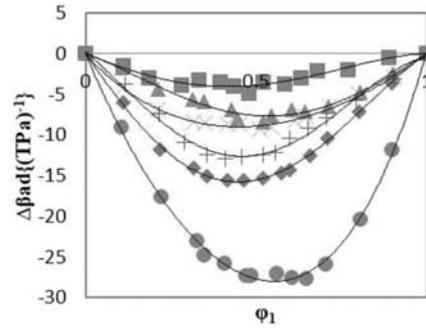


Fig. 12 Deviations in adiabatic compressibilities ($\Delta\beta_{ad}$) with volume fractions (ϕ_1) of 1, 4-dichlorobutane for binary mixtures of 1, 4-dichlorobutane + cyclohexane (\bullet), + benzene (+), + methylbenzene (\blacklozenge), + 1, 2-dimethylbenzene (\blacksquare), + 1, 4-dimethylbenzene (\times) and + 1, 3, 5-trimethylbenzene (\blacktriangle) at temperature 318.15K. The points represent experimental values calculated from Eq. (5) and line represent R - K values calculated from Eq. (6).

where n is the total number of experimental points and m is the number of coefficients in Eq. (6). The values of $\sigma(\Delta\beta_{ad})$ are also recorded in Table 1 along with the coefficients.

Perusal of Figs. 10-12 shows that $\Delta\beta_{ad}$ values are negative for all the binary mixtures at the three experimental temperatures. The algebraic values of $\Delta\beta_{ad}$ for equi-volume fraction mixtures *i.e.* at $\Phi = 0.5$ for all the six binary mixtures at the three experimental temperatures follow the order:

Table 1 – Values of the coefficients a_0, a_1, a_2, \dots of Redlich - Kister polynomial equation and standard deviations in deviation in adiabatic compressibility $\sigma(\Delta\beta_{ad})$ (all in $\{(TPas)^{-1}\}$) for the binary systems at different temperatures 308.15K, 313.15K and 318.15K.

T/K	a_0	a_1	a_2	a_3	a_4	$\sigma(\Delta\beta_{ad})$
1, 4-dichlorobutane (x_1) + cyclohexane (x_2)						
308.15	-104.7440	-21.1720	-8.9077	7.1581	23.2565	0.6315
313.15	-103.5480	-34.5869	-7.8388	13.6945	31.6269	0.2867
318.15	-109.6180	-22.4475	-38.1612	1.4403	52.3185	0.4488
1, 4-dichlorobutane (x_1) + benzene (x_2)						
308.15	-50.0012	21.1887	24.2206	-39.0388	2.9244	0.2202
313.15	-47.8133	19.9661	21.2035	-29.2773	8.1304	0.2132
318.15	-50.4230	22.7551	35.8021	-37.9563	-15.6635	0.2929
1, 4-dichlorobutane (x_1) + methylbenzene (x_2)						
308.15	-54.5673	22.2119	14.3733	-16.2852	6.4492	0.3067
313.15	-48.6709	21.1399	21.0741	-39.6848	26.1690	0.2005
318.15	-62.0444	18.7971	13.8301	-6.5797	8.8369	0.3263
1, 4-dichlorobutane (x_1) + 1, 2-dimethylbenzene (x_2)						
308.15	-22.2967	-2.0143	4.2390	-6.5788	6.9122	0.4235
313.15	-28.1932	2.2110	23.0120	-5.4010	-14.9756	0.5216
318.15	-15.1808	7.9286	-0.0188	-0.7731	13.7129	0.5589
1, 4-dichlorobutane (x_1) + 1, 4-dimethylbenzene (x_2)						
308.15	-44.7050	7.3828	-4.1219	1.7068	10.0360	0.2583
313.15	-42.2203	3.1252	1.9776	5.2226	-5.1602	0.2177
318.15	-35.9108	6.0769	3.3527	2.7323	-13.0917	0.2717
1, 4-dichlorobutane (x_1) + 1, 3, 5-trimethylbenzene (x_2)						
308.15	-16.1629	17.2228	-1.9863	-27.5177	4.2589	0.4759
313.15	-28.9457	-5.8912	8.3494	5.7427	-12.1736	0.5425
318.15	-30.3083	-5.2127	7.1355	-1.6362	5.5679	0.4854

At 308.15 K : 1, 3, 5-trimethylbenzene > 1, 2-dimethylbenzene > 1, 4-dimethylbenzene > benzene > methylbenzene > cyclohexane

At 313.15 K : 1, 2-dimethylbenzene > 1, 3, 5-trimethylbenzene > 1, 4-dimethylbenzene > benzene > methylbenzene > cyclohexane

At 318.15 K : 1, 2-dimethylbenzene > 1, 3, 5-trimethylbenzene > 1, 4-dimethylbenzene > benzene > methylbenzene > cyclohexane

It has been suggested⁹⁻¹⁰ that expansibility of the mixture of two liquids depends on following factors: (i) loss of dipolar association in polar molecule on addition of second components. (ii) interactions between unlike molecules due to dipole - induced dipole, dipole- dipole and charge - transfer interactions and (iii) molecular packing which depends on the size and shape of the molecules of the components of the mixture.

The factor (i) contributes to increase in free length. This in turn causes positive deviation in adiabatic compressibility¹¹. The (ii) factor, on the other hand, contributes to a negative deviation in adiabatic compressibility. The (iii) factor may contribute to adiabatic compressibility in two ways. If the size and shape of the molecules of the second component is such that, it locks into the voids created by the molecules of the first component, the deviation in adiabatic compressibility is negative. On the other hand, if due to size and shape of the molecules, the second component may blocks to approach of the first component, the deviation in adiabatic compressibility may become positive.

1, 4-dichlorobutane is a polar molecule having dipole moment 2.22D¹². In liquid state it remains in self-associated form due to dipolar interactions between the molecules. When binary mixture is prepared with aromatic hydrocarbons having six membered ring with

polarizable π -electrons, dipole - induced dipole interactions take place and due to (ii) factor, a negative deviations in adiabatic compressibility as in our case is observed. Cyclohexane with a six membered ring having no π -electrons should contribute according to factor (i). However, in our case, the binary mixture of 1, 4-dichlorobutane + cyclohexane has a large negative deviations in adiabatic compressibility. It seems that the sign and magnitude of the $\Delta\beta_{ad}$ values depends on relative strengths of several contributing factors.

The methylbenzene and 1, 2-dimethylbenzene are polar molecules with dipole moment values¹² 0.37D and 0.62D respectively. The binary mixtures of 1, 4-dichlorobutane with these two aromatic hydrocarbons should have more negative values of $\Delta\beta_{ad}$ due to stronger dipole - dipole molecular interactions than the binary mixtures with benzene having a dipole - induced dipole interactions. However, in our case the $\Delta\beta_{ad}$ values for binary mixture of 1, 4-dichlorobutane + 1, 2-dimethylbenzene has the reverse trend. It may be due to several opposing contributions which modify the actual values.

Conclusions

The ultrasound velocity (u) in binary mixtures of 1, 4-dichlorobutane + cyclohexane increase with increase in molefractions of 1, 4-dichlorobutane. ' u ' values decrease with increase in molefractions of 1, 4-dichlorobutane for binary mixtures prepared with aromatic hydrocarbons. Adiabatic compressibility decrease for all the binary mixtures with increase in mole fractions of 1, 4-dichlorobutane. Deviations in adiabatic compressibility, $\Delta\beta_{ad}$ are negative for all the binary systems studied.

Acknowledgments

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Study of physical and acoustical properties of nuclear extractant

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Solvent extraction is largely applied in the purification in chemical and hydrometallurgical industries. The selection of proper extractants with a suitable diluents cause an efficient extraction of different metals from their components. The separation technology follows different method for extraction of the metals from ionic solution using various properties. But all the methods have various drawbacks in respect of technology or cost factor. After all, ultrasonic technique is one of the best and cheapest procedures for analysis of solvent extraction using different extractants with diluents. The present work deals with the study of some physical and acoustical properties like density, viscosity, ultrasonic velocity and compressibility *etc.* in the tributyl phosphate (TBP)-benzene system at temperature 30°C, 35°C and 40°C. The variations of different physical and acoustical properties are discussed in terms of interaction which has been well explained the solubility of the extractants for solvent extraction.

Keywords: Ultrasonic velocity, extractants, diluents, acoustical properties, acoustical parameter.

Introduction

The commercial use of the tributyl phosphate (TBP), particularly in the nuclear fuel reprocessing industry has led to the development of many analytical methods for the determination of concentration of TBP and its degradation products¹⁻². The methods for estimation mostly include paper, thin layer, gas and liquid chromatography. Different authors have developed analytical techniques to determine the concentration of TBP in hydrocarbon diluents. Among them the ultrasonic technique is the most easy and accurate estimation of extractant and diluents pair used for nuclear industry. Being ultrasonic wave a sub category of acoustics it has high frequency- low intensity and low frequency - high intensity which makes it possible to obtain the information about the medium or to convey information through the medium through molecular interactions between the molecules of the medium. The wavelength of this wave changes from one medium to another medium due to which it can be reflected off with very small surfaces and provides information from atomic/subatomic level. Diluent plays a very important role in the extraction. The rate of extraction depends upon the

nature of the diluents and temperature of the system. The properties like density, viscosity *etc.* play a deciding role in extraction. The extraction of TBP has been carried out using aromatic hydrocarbon like benzene. The extracting power of TBP is mainly due to presence of phosphoryl group which form adducts or solvates with the metal ions. The physical properties like viscosity, density, solubility surface tension play a very important role in solvent extraction studies. TBP is generally used in conjunction with hydrocarbon diluents which is inert in nature. The diluent like benzene improves the physical properties of TBP by lowering the density and viscosity for better phase separation³. Hence, it is important to study various physical properties of TBP in presence of diluent.

Materials and Methods

High purity and analytical grade samples of TBP 99.05 (GC) and benzene 99.0% (GC) are procured from CDH chemicals India. The entire chemical used in the study are purified by standard procedure⁴⁻⁵ and redistilled before use. To minimize the contact of this deliquescent reagent with moist air, the product was kept in sealed

bottles in desiccators. The purities of the sample were confirmed by GLC. Binary mixtures were prepared by mass in air tight bottles. The mass measurements were performed on high precision digital balance with an accuracy of + 1 mg. The uncertainty in mole fraction was + 0.0001. The densities of pure liquids and their mixture were determined by using double arm pycnometer with accuracy of the order of + 0.01 kg/m³.

Experimental

The ultrasonic speed of the above liquids and their mixtures were measured using multi-frequency ultrasonic interferometer operating at different frequencies like 1 MHz, 3 MHz and 5 MHz. The accuracy in the measurement of ultrasonic velocity was within ± 0.01 ms⁻¹. The working principle used in the measurement of velocity of sound through medium was based on the accurate determination of the wave length of ultrasonic waves of known frequency produced by quartz crystal in the measuring cell⁶⁻⁷. The temperature of the solution was controlled by circulating water at a desired temperature through the jacket of double walled cell within ± 0.01 K using a constant temperature bath with an accuracy of ± 0.001 K.

Theory

The experimental measured values of ultrasonic speed and computed values of density are used to compute acoustic parameters such as intermolecular free length (L_f), isentropic compressibility (β), acoustic impedance (Z) their excess values. The above acoustic parameters are determined with the help of the following relationship

$$\text{Isentropic compressibility } (\beta_s) = \frac{1}{\rho C^2} \quad (1)$$

$$\text{Intermolecular free length } (L_f) = k\beta^{1/2} \quad (2)$$

$$\text{Acoustic impedance } (Z) = \rho C \quad (3)$$

where C is the ultrasonic velocity and their excess values are calculated as $(Y^E) = Y_{mix} - (X_A Y_A + X_B Y_B)$ (4)

where X_A , X_B , Y_A , Y_B and Y_{mix} are mole fraction, isentropic compressibility, inter molecular free length, acoustic impedance of benzene, TBP and mixture respectively. The constant k is temperature dependent which is given as $[93.875 + (0.375T)] \times 10^{-8}$ as per literature⁸ and T being the absolute temperature.

Results and Discussion

The computed values of density of the mixture and measured values of ultrasonic are used to calculate the different acoustic parameters and their excess values are shown in Figs. 1-5. It is seen that the ultrasonic velocity decreases with increasing mole fraction of TBP, depending on the ultrasonic velocity value of second component in the entire sample as shown in Fig. 1. The effect of adding a non-polar second component is primarily to disrupt the dipolar interactions of the first component. This may be due to self association of the solvent molecules and a very weak dipole-induced dipole interaction between the component molecules, which is concentration dependent⁹. Again, with increase of temperature the ultrasonic velocity decreases with increasing values of mole fraction of TBP due to having negative temperature gradient of velocity.

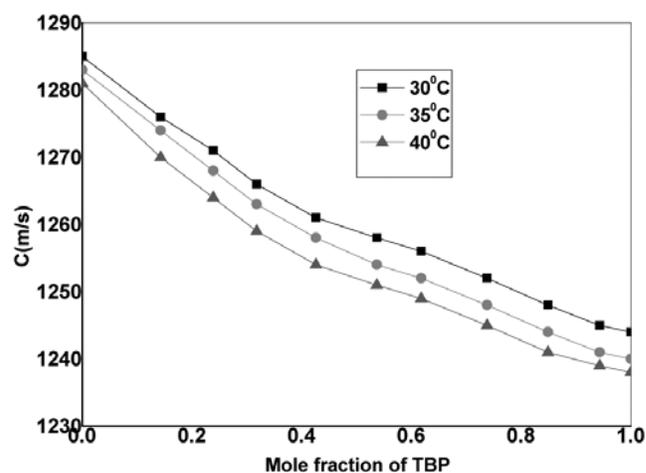


Fig. 1 Variation of ultrasonic velocity with temperature

As isentropic compressibility (β) varies inversely with C^2 , the trend in isentropic compressibility with concentration is the reverse of the trend in ultrasonic velocity with concentration. Further, the plots of isentropic compressibility with concentration of TBP are non linear suggesting that these systems are deviated from the ideal ones. The variations in isentropic compressibility values with concentration indicate that the strength of induced dipole-induced dipole interactions is concentration dependent as shown in Fig. 2. The variation of ultrasonic velocity in a solution depends upon the increase or decrease of intermolecular free length after mixing the components.

From Fig. 3 it is clear that the value of excess compressibility and intermolecular free length becomes more

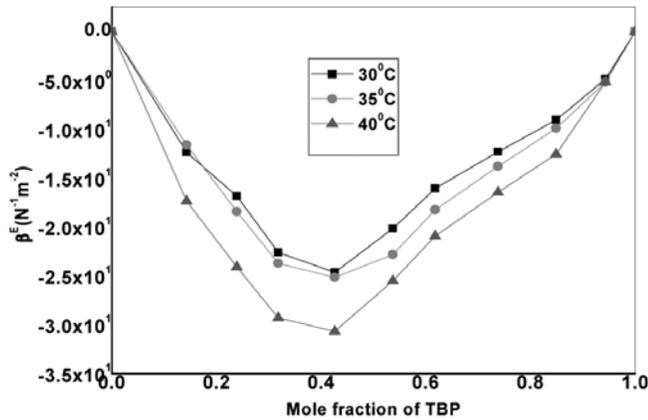


Fig. 2 Variation of excess isentropic compressibility

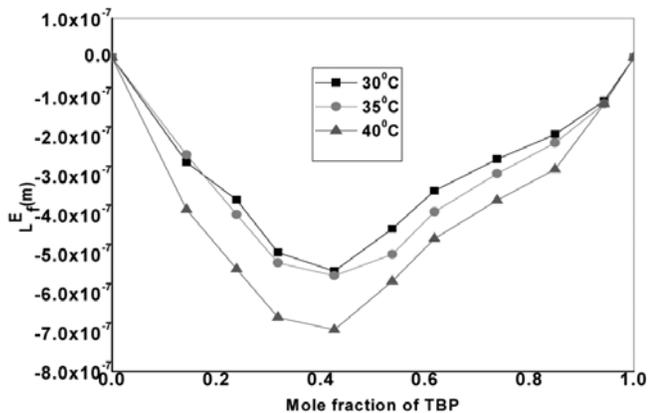


Fig. 3 Variation of excess intermolecular free length

negative with increase of temperature. This behaviour indicates that the strength of interaction between unlike molecules in the present study increases with temperature in the binary mixture. According to Fort and Moore a negative excess compressibility is an indication of strong hetero molecular interaction in the liquid mixtures which is attributable to charge transfer, dipole-dipole, and dipole-induced dipole interaction and is attributed to dispersion forces.

The variation of β^E and L_f^E are also supported by existence of some specific interaction like excess values of acoustic impedance Z^E . The variation of Z^E as shown in Fig. 4 in the system reveals that dispersion is more prominent in the systems but the less magnitude of Z^E suggests that there is possibility of weak dipole-induced dipole type of interaction acting between system components. From the nature of the profile it is very clear that in TBP and benzene system the magnitude of Z^E is appreciably more negative suggesting the fact that

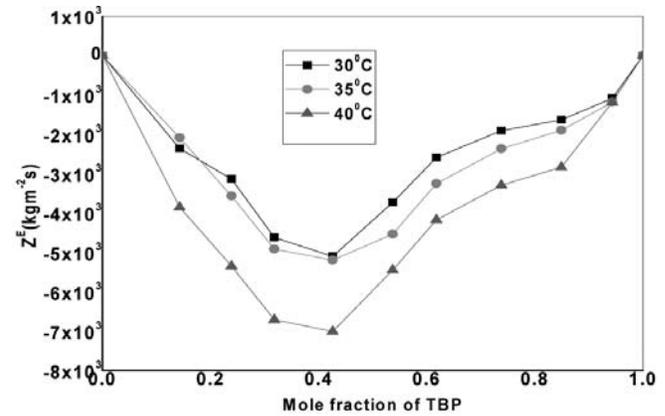


Fig. 4 Variation of excess acoustic impedance

the dispersion is more prominent and having weak dipole-induced dipole interaction in the system.

With increase of temperature the values of Z^E is more negative indicates that the system is less resistive to propagation of ultrasonic wave.

From the Fig. 5 it is clear that the surface tension increases with increase of TBP and decreases with increases of temperature. This indicates that with increase of temperature the particles execute random motion for which the medium become less dense. As a result the density of the medium decreases indicating high degree of extraction processes¹⁰⁻¹¹.

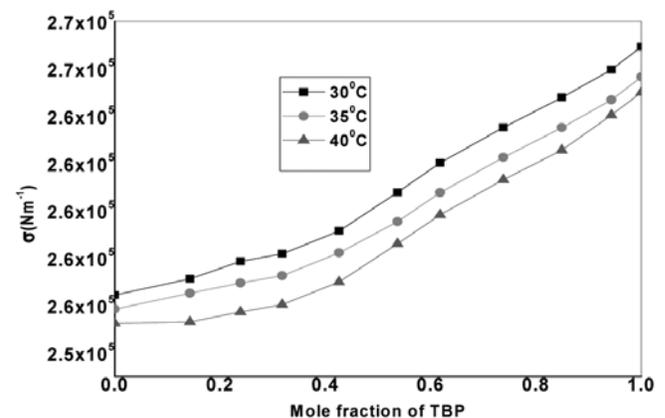


Fig. 5 Variation of surface tension

Conclusions

Thus it can be concluded that the interaction of TBP with benzene is stronger in high temperature as is observed in different acoustic parameters for different

temperature. The dependence of ultrasonic velocity and other derived parameters on composition of the mixture is indicative of the presence of molecular interactions. The sign and magnitude of excess parameter of the mixture and their variations with temperature reveals that the extent of interaction increases with increase in temperature. When the concentration of benzene decreases and TBP concentration increases there is more than one type interaction like dipole-dipole, dipole-induced dipole, dispersion force may appears in the mixture which basically explains the dissociation of organo-aquo phase of dissolved rare earth element in extraction process which may lead to key issue in extraction technology.

Acknowledgments

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Ultrasonic investigations of molecular interaction in binary mixtures of ellagic acid with acetone

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The generated ultrasonic wave for a particular frequency (2 MHz) affects the molecular interaction of binary mixture of ellagic acid in acetone. Ellagic acid is a powerful bioactive compound with many potential pharmacological and industrial applications. Ellagic acid is a polyphenolic compound in fruits and berries. The experimental data have been used to compute some acoustic and thermodynamic parameters such as adiabatic compressibility, intermolecular free length, free volume, relaxation time and acoustic impedance at different temperature over the entire composition range. The non-linear variations of these derived acoustical parameters with different concentration of the solute explained on the basis of structural changes occurring in a solution. The variation in ultrasonic velocity and other parameters play an important role in understanding solute-solvent interaction between the constituent molecules are presented with some possible reasons.

Keywords: Ellagic acid, relaxation time, free volume.

Introduction

The molecular interactions among the various components of the binary mixtures can be studied by using thermodynamic and acoustic properties of ellagic acid in acetone. Ellagic acid is a type of hydrolysable tannin. In different plant species Tannin is polyphenolic compound. Tannins astringent, bitter plant polyphenols that either bind and precipitate or shrink proteins. The astringency from the tannins is that which causes the dry and puckery feeling in the mouth following the consumption of red wine, strong tea, or an unripened fruit¹.

Ellagic acid is used for the commercial purpose due to its benefits to human health, properties and application in various fields. The presence of ellagic acid in a range of commercial products giving antioxidant activity has also been reported. These molecules have a variety of benefits for their anti-mutagenic, antimicrobial and antioxidant properties, and inhibitors of human immunodeficiency virus (HIV). Ellagic acid used as an antiviral and antimicrobial agent². Ellagic acid ($C_{14}H_6O_8$) is a rich source from certain fruits and nuts

including grapes, strawberries, raspberries, pomegranate, morinda citrifolia, terminalia chebula and walnut. This phenol is one of the most promising chemo preventive agents³.

Acetone belongs to the carbonyl compound series having functional group $C=O$ and it has the ability to dissolve other materials and organic solvents. Acetone is also a useful solvent in the pharmaceutical industry; it can be used as a chemical intermediate and a solvent for vitamins and cosmetic products.

Data like density, viscosity, ultrasonic velocity and some other thermodynamic parameters find some widespread applications in chemical engineering processes, textile industries and molecular dynamics⁴⁻⁶.

In the present study measurements of densities, viscosity and speed of sound for ellagic acid and acetone at various temperatures 298K, 303K, 308K, and 313K at various molar concentrations in the range of 0.01 mol to 0.09 mol is carried out. Based on these values and using various formulae, a few thermo-acoustical parameters at different temperature were derived over

the entire composition range. Results are used to explain the nature of molecular interactions between mixing compounds.

Materials and Methods

AR grade chemicals are used for the preparation of liquid mixture of various concentrations in mole fraction. The study was carried out for the fixed frequency 2MHz of ultrasonic cell at various temperatures 298K, 303K, 308K and 313K. During observation temperature of the binary liquid mixture is kept constant within an accuracy of $\pm 0.1^\circ\text{C}$ by using thermostat. Viscosity measurements were taken using Ostwald's viscometer with an accuracy of $\pm 0.1 \text{ kg/m}^3$. The density of the solution was determined accurately using 10 ml specific gravity bottle and electronic balance and accuracy in the density measurement is $\pm 1 \times 10^{-5} \text{ g/cm}^3$.

Ultrasonic velocity is noted by an ultrasonic multi frequency interferometer operating at a frequency range 1 MHz to 10 MHz with an accuracy of $\pm 0.01 \text{ m/s}$. The source of ultrasonic waves was a quartz crystal excited by a radio frequency oscillator. The cell was filled with desired solution and water at constant temperature was circulated in the outer jacket.

Results and Discussion

Figure 1 shows the plot of density against molar concentration in which density increases with increase in molar concentration of binary liquid but decreases with increase in temperature. Increase in density decreases the free volume indicating association in component molecules.

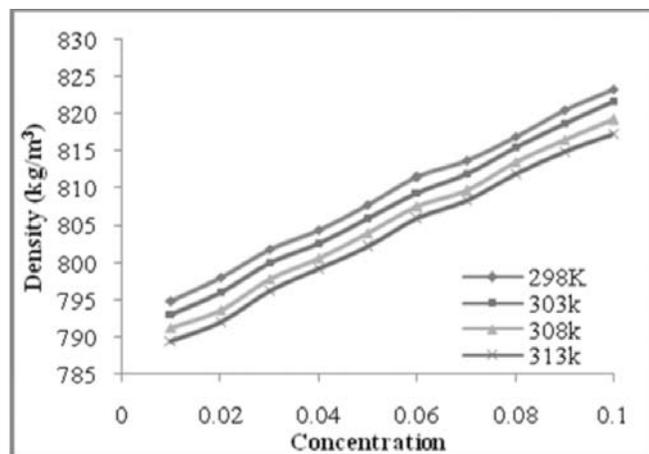


Fig. 1 Variation of density with molar concentration of acetone.

Figure 2 contains the plot of ultrasonic velocity versus molar concentration. The non linear variation in velocity gives information about the binding between the molecules and formation of complexes at various temperatures through molecular interactions⁷.

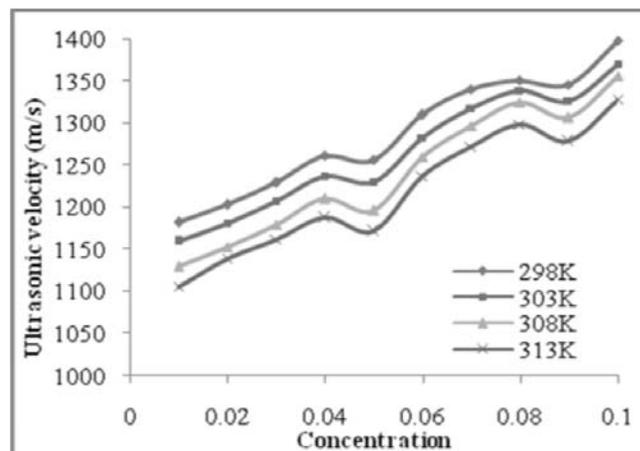


Fig. 2 Variation of ultrasonic velocity with molar concentration of acetone.

Measurements of viscosity in binary liquid mixture yield some reliable information in the study of molecular interaction⁴. Viscosity decreases with increase in temperatures as shown in Fig. 3.

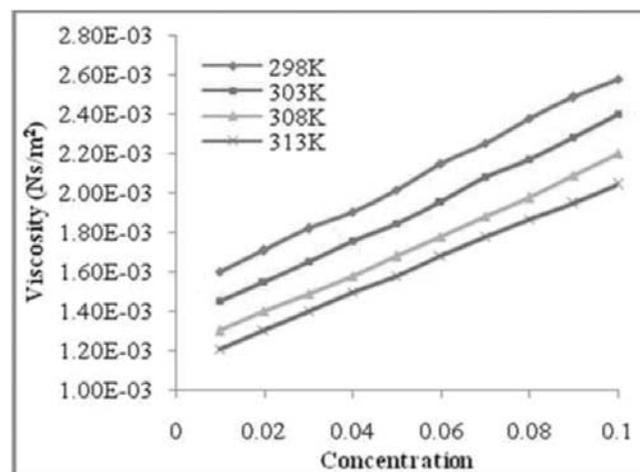


Fig. 3 Variation of viscosity with molar concentration of acetone.

The decrease of adiabatic compressibility with increase in concentration of ellagic acid in acetone as shown in Figure 4 indicates there is definite contraction in the components molecules⁸.

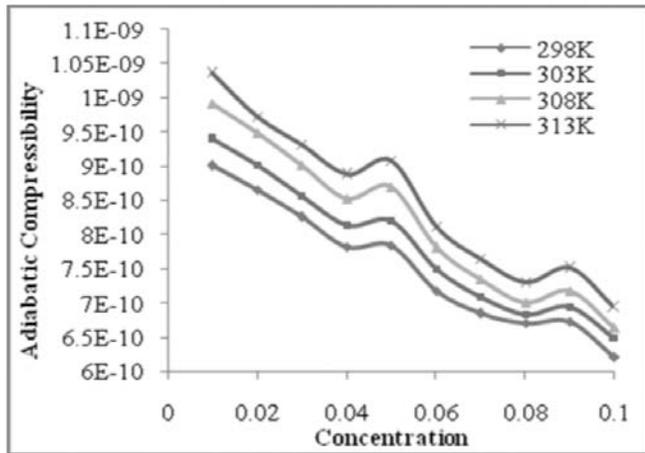


Fig. 4 Variation of adiab. compressibility with molar concentration of acetone.

Figure 5 contains the plot of free length versus molar concentration. Free length decreases ultrasonic velocity increases showing an inverse behavior, it is in good agreement with theoretical results⁹.

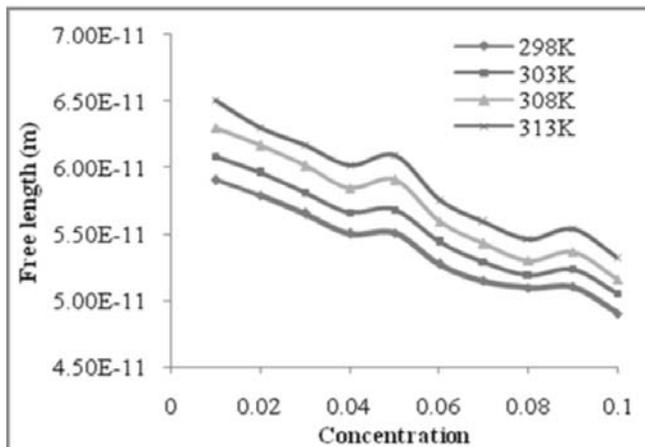


Fig. 5 Variation of free length with molar concentration of acetone.

Figure 7 illustrates the variation of acoustic impedance with molar concentration. The increase in specific acoustic impedance indicates significant interaction between the mixing components¹⁰.

Figure 8 contains the plot of relaxation time (τ) versus molar concentration. It is observed that relaxation time increases with increase in molar concentration of ellagic acid in acetone indicating more stability of ellagic acid molecules¹¹.

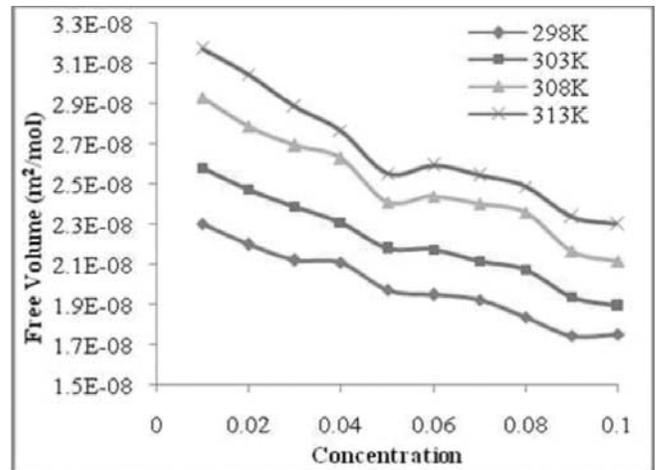


Fig. 6 Variation of free volume with molar concentration of acetone.

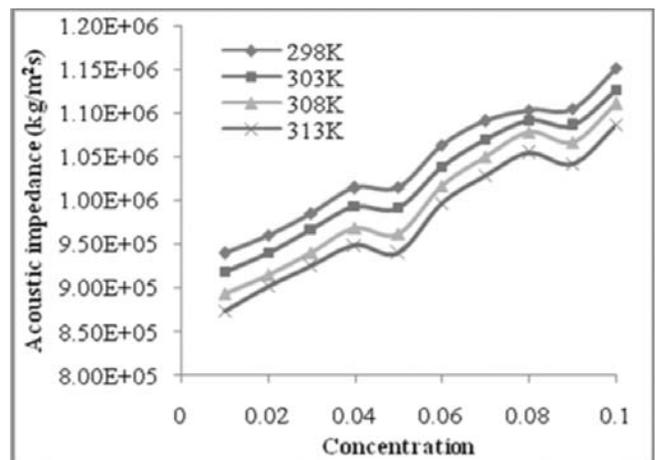


Fig. 7 Variation of acoustic impedance with molar concentration of acetone.

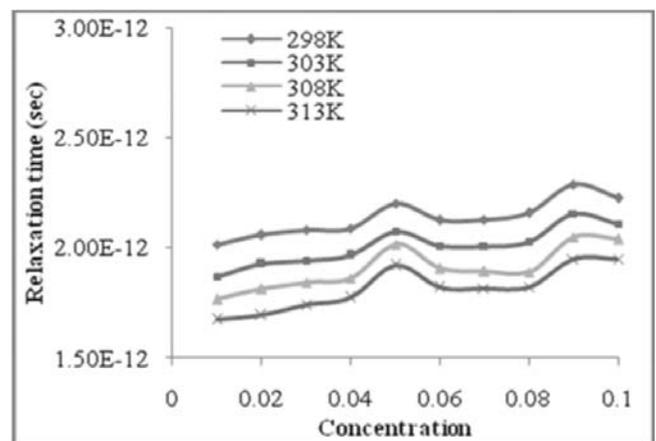


Fig. 8 Variation of relaxation time with molar concentration of acetone.

Conclusions

The variation of acoustical parameters derived from ultrasonic velocity, density and viscosity suggest that the presence of molecular interaction between component of molecules in the binary liquid mixture.

An analysis of these values suggests the presence of strong intermolecular interaction in the binary mixtures which may be due to hydrogen bond, or due to interstitial accommodation in the constituent's molecules.

The nonlinear variation of thermo acoustic parameters with molar concentration provides valuable information about the strength of molecular interactions in the binary liquid mixture.

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Elastic and acoustic properties of hexagonal intermetallic ternary compound

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The elastic, acoustic and mechanical properties of the hexagonal AlB_2 -type intermetallic NdCuGe ternary compound have been studied along unique axis at room temperature. The second- and third order elastic constants have been calculated for NdCuGe compound using Lennard-Jones potential model. The temperature variation of the ultrasonic velocities is evaluated along different angles with unique axis of the crystal using the second order elastic constants. Temperature variation of the thermal relaxation time and Debye average velocities is also calculated along the same orientation. The temperature dependency of the acoustic properties is discussed in correlation with elastic, thermal and electrical properties. It has been found that the thermal conductivity is the main contributor to the behaviour of ultrasonic attenuation as a function of temperature and the responsible cause of attenuation is phonon-phonon interaction. The mechanical properties of NdCuGe intermetallic compound at low temperature are better than at room temperature, because at low temperature it has low ultrasonic velocity and ultrasonic attenuation.

Keywords: Elastic properties, thermal conductivity, acoustic properties, ternary intermetallic compounds.

Introduction

The ternary rare-earth compounds in $R-T-X$ systems, where R =rare earth metals, T = transition metals and X = Si , Ge , have received strong attention in recent years because of their important role in many technological applications such as microwave devices, permanent magnets, and magnetic and optical recording devices. Thus, new ternary compounds with superior properties have been intensively explored. Previous study of the Nd-Cu-Ge system reported five ternary compounds with distinct structures¹. The magnetic properties of NdCuGe have also been investigated, and the results have indicated the Curie-Weiss paramagnetic behaviour for all compounds at high temperatures². It is well known that rare-earth based compounds exhibit a variety of magnetic behaviour depending on the ratio of exchange interactions to crystal field interactions. The ternary equiatomic lanthanide germanides have been extensively studied³. NdCuGe intermetallic compound have hexagonal crystal structures with the AlB_2 type structure (space group designation $P6/mmm$)⁴.

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 constants⁵. The elastic constants provide valuable information about the bonding characteristic between adjacent atomic planes and the anisotropic character of the bonding and structural stability⁶.

Given the aforementioned potential applications, the complete knowledge of mechanical and physical properties of NdCuGe, however, is still lacking. For example, the non-linear elastic mechanical properties such as elastic constants, attenuation *etc.* has not been addressed yet, therefore, in present work predict the ultrasonic properties of NdCuGe at different temperatures. The ultrasonic attenuation coefficient, acoustic coupling constants, higher order elastic constants, thermal relaxation time and ultrasonic wave velocities for NdCuGe for unique direction of propagation of wave are calculated as a function of

temperature. The calculated ultrasonic parameters are discussed with related thermophysical properties for the characterization of the chosen ternary intermetallic compound.

Theory

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

$$C_{IJ} = \frac{\partial^2 U}{\partial e_i \partial e_j}; \quad \text{I or J} = 1, \dots, 6 \quad (1)$$

$$C_{IJK} = \frac{\partial^3 U}{\partial e_i \partial e_j \partial e_k}; \quad \text{I or J or K} = 1, \dots, 6 \quad (2)$$

where, U is elastic energy density, $e_I = e_{ij}$ (i or $j = x, y, z$, $I = 1, \dots, 6$) is component of strain tensor. Eqs (1) and (2) leads six second and ten third order elastic constants (SOEC and TOEC) for the hexagonal structure materials⁷.

The expressions for ultrasonic attenuation, ultrasonic velocities and allied parameters are given in our previous papers^{8, 9}.

Results and Discussion

Higher order elastic constants

The lattice constants *i.e.* the unit cell parameters ' a ' (basal plane parameter) and ' p ' (axial ratio) for NdCuGe, are 4.277Å and 0.907 respectively¹⁰. The value of ' m ' and ' n ' for NdCuGe ternary compound are 6 and 7. The value of b_0 for NdCuGe is 4.2×10^{-63} erg cm⁷. The second order elastic constants (SOEC) and third order elastic constants (TOEC) have been calculated for NdCuGe compound and bulk modulus (B) are presented in Table 1.

The elastic constants of the material are important, since they are related to hardness and therefore of interest in applications where mechanical strength and durability

are important. Also, the second order elastic constants are used for the determination of the ultrasonic attenuation and related parameters. The comparison can be made with the value of Debye temperature of NdCuGe compound. The present value of Debye temperature for NdCuGe is 243K, which has been computed using second order elastic constants. The Debye temperature of NdCuGe is 240K, which has determined by Goruganti *et.al.*¹⁰. Since the Debye temperature has evaluated with ultrasonic velocities and ultrasonic velocities is depending on second order elastic constants. 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 our previous papers for hexagonal structure materials¹¹. Hence applied theory for the evaluation of higher order elastic constants at room temperature is justified. Also, the bulk modulus (B) for NdCuGe can be calculated with the formula $B = 2(C_{11} + C_{12} + 2C_{13} + C_{33})/9$. The evaluated ' B ' for NdCuGe is presented in Table 1. To satisfy the conditions of the mechanical stability following criteria¹²: $C_{11} > C_{12}$; $(C_{11} + C_{12}) C_{33} > 2C_{13}^2$; $C_{44} > 0$; $C_{66} > 0$ on the elastic constants must be fulfilled. As our calculated results for elastic constants reasonably satisfy aforesaid criteria for the intermetallic ternary NdCuGe compound which indicate that this compound is mechanically stable.

Ultrasonic velocity and allied parameters

The temperature dependent electrical resistivity of intermetallic ternary NdCuGe compound has been taken from the previous work¹⁰. The thermal conductivity of NdCuGe compound is evaluated using electrical resistivity. The value of C_V and E_0 are evaluated using tables of physical constants and Debye temperature. The value of temperature dependent density (ρ), specific heat per unit volume (C_V), thermal energy density (E_0), thermal conductivity (k) and calculated acoustic coupling constants (D_L and D_S) are presented in Table 2.

The computed orientation dependent ultrasonic wave velocities and Debye average velocities at room temperature are shown in Figs. 1-4. Figs. 1-4 show that

Table 1 – SOEC, TOEC and bulk modulus (B) in the unit of 10^{10} Nm⁻² of NdCuGe compound at room temperature.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B			
NdCuGe	47.65	11.70	3.13	4.64	3.76	18.69	4.56			
	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{344}	C_{144}	C_{155}	C_{222}	C_{333}
NdCuGe	-777.06	-123.20	-8.04	-10.22	-15.68	-14.71	-11.90	-7.93	-614.83	-18.16

Table 2 – Density (ρ : in 10^3 kg m^{-3}), specific heat per unit volume (C_V : in $10^5 \text{ Jm}^{-3}\text{K}^{-1}$), thermal energy density (E_0 : in 10^6 Jm^{-1}), thermal conductivity (k : in $\text{Wm}^{-1}\text{K}^{-1}$) and acoustic coupling constant (D_L, D_S) of NdCuGe compound.

Temp. (K)	ρ	C_V	E_0	k	D_L	D_S
50	7.62	2.636	4.308	1.371	16.819	20.81
100	7.60	5.156	25.725	1.952	16.833	20.81
150	7.58	5.960	54.493	2.259	16.837	20.81
200	7.56	6.273	83.561	2.477	16.839	20.81
250	7.54	6.426	116.315	2.699	16.841	20.81
300	7.52	6.509	146.979	2.815	16.842	20.81

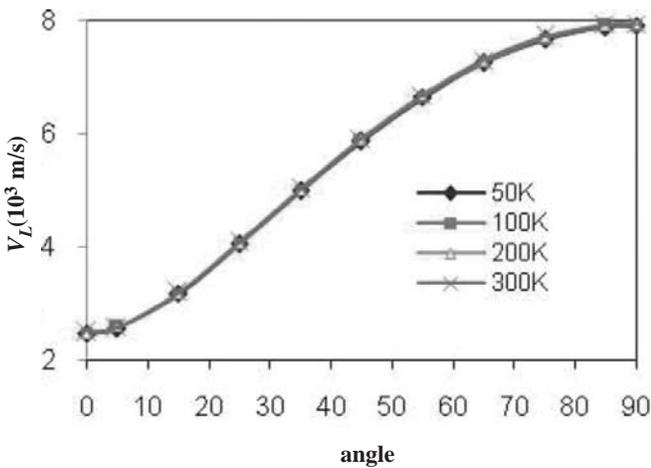


Fig. 1 V_L vs angle with unique axis of crystal

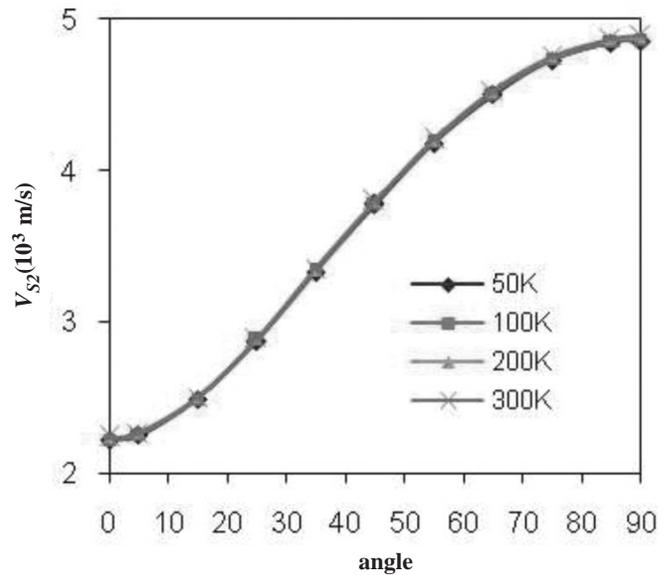


Fig. 3 V_{S2} vs angle with unique axis of crystal

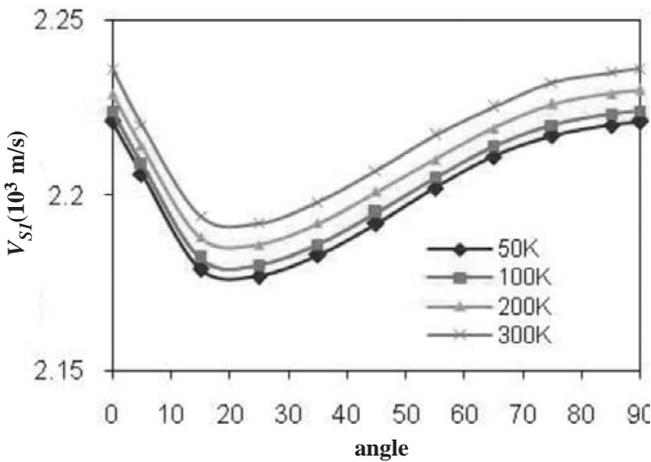


Fig. 2 V_{S1} vs angle with unique axis of crystal

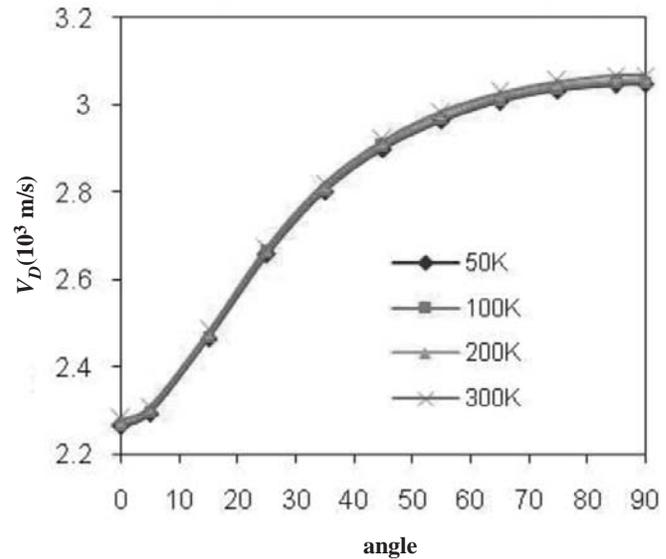


Fig. 4 V_D vs angle with unique axis of crystal

the velocities V_L , V_{S2} and V_D increase with the angle from the unique axis and V_{S1} have minimum at 25° with the unique axis of the crystal. The combined effect of SOEC and density is reason for abnormal behaviour of angle dependent velocities.

The nature of the angle dependent velocity curves in the present work is found similar as that for ceramics materials, semiconducting materials and other hexagonal structured materials^{5,8,11}. Thus the angle dependencies of the velocities in NdCuGe are justified.

Debye average velocity of NdCuGe is increasing with the angle from the unique axis at room temperature (Fig. 4). Since V_D is calculated using V_L , V_{SI} and V_{S2} ,⁹ therefore the angle variation of V_D is influenced by the constituent ultrasonic velocities. The increase in V_D at unique axis of crystal is due to significant increases in longitudinal and quasi-shear (V_{S2}) wave velocities and a variable pure shear (V_{SI}) wave velocity. Thus it can be concluded that when a sound wave travels at 90° with the unique axis of these crystals then the average sound wave velocity is maximum and minimum at 0° with unique axis.

The calculated thermal relaxation time is visualized in Fig. 5. The angle dependent thermal relaxation time curves follow the reciprocal nature of V_D as $\tau \propto 3k/C_V V_D^2$. This implies that ' τ ' for chosen compound is mainly affected by the thermal conductivity. The ' τ ' for hexagonal structured materials is the order of pico second⁵. Hence the calculated ' τ ' justifies the hexagonal structure of chosen ternary compound. The minimum thermal relaxation time for wave propagation along $\theta = 90^\circ$ implies that the re-establishment time for the equilibrium distribution of thermal phonons will be minimum for propagation of wave along this direction. Thus the present average sound velocity directly correlates with the Debye temperature, specific heat and

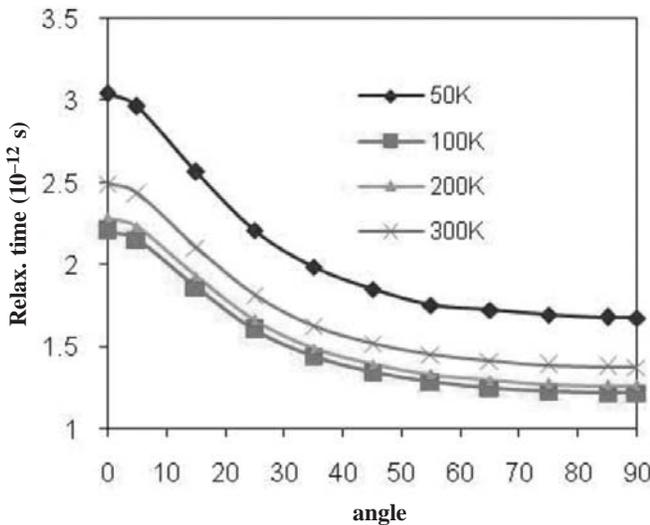


Fig. 5 Relaxation time vs angle with unique axis of crystal

thermal energy density of NdCuGe.

Ultrasonic attenuation due to phonon-phonon interaction and thermal relaxation phenomena

In the evaluation of ultrasonic attenuation, it is supposed that wave is propagating along the unique axis [$<001>$ direction] of NdCuGe. The attenuation coefficient over frequency square $(A/f^2)_{Akh}$ for longitudinal $(A/f^2)_L$ and shear wave $(A/f^2)_S$ are calculated under the condition $\omega\tau \ll 1$ at different temperature. The values of temperature dependent $(A/f^2)_L$, $(A/f^2)_S$, $(A/f^2)_{Th}$ and total attenuation $(A/f^2)_{Total}$ are presented in Figs. 6-7.

In the present investigation, the ultrasonic wave propagates along the unique axis of the crystal, the Akhieser type of loss of energy for longitudinal and shear wave and thermo elastic loss increases with the temperature of the material (Figs. 6-7). $(A/f^2)_{Akh}$ is proportional¹¹ to D , E_0 , τ and V^{-3} . The E_0 is increasing with the temperature (Fig. 1-4). Hence, Akhieser loss in NdCuGe is predominantly affected by the thermal energy density E_0 and the thermal conductivity.

Therefore, the ultrasonic attenuation decreases due to the reduction in the thermal conductivity. Thus ultrasonic attenuation is mainly governed by the phonon-phonon interaction mechanism. A comparison of the ultrasonic attenuation could not be made due to lack of experimental data in the literature.

Figures 6-7 indicate that the thermoelastic loss is very small in comparison to Akhieser loss and ultrasonic

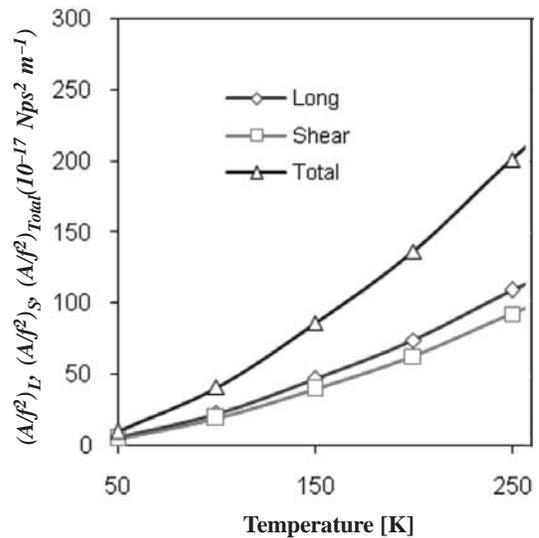


Fig. 6 $(A/f^2)_{Total}$ and $(A/f^2)_{Akh}$ vs temperature of NdCuGe

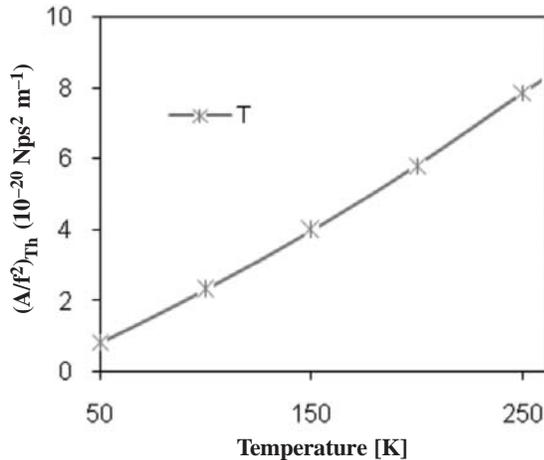


Fig. 7 $(A/f^2)_{Th}$ vs temperature of NdCuGe

attenuation for longitudinal wave $(A/f^2)_L$ is greater than that of shear wave $(A/f^2)_S$. This reveals that ultrasonic attenuation due to phonon-phonon interaction along Akhieser loss is governing factor for total attenuation $((A/f^2)_{Total} = (A/f^2)_{Th} + (A/f^2)_L + (A/f^2)_S)$. The total attenuation is mainly affected by thermal energy density and thermal conductivity. Thus it may predict that at 50K the *NdCuGe* behaves as its purest form and is more ductile as evinced by minimum attenuation while at room temperature *NdCuGe* is least ductile. Therefore impurity will be least in the *NdCuGe* at low temperature (50 K). The minimum ultrasonic attenuation for *NdCuGe* at 50 K justifies its quite stable hexagonal structure state. The total attenuation of *NdCuGe* is larger than third group nitrides (AlN: $4.441 \times 10^{-17} \text{ Nps}^2 \text{ m}^{-1}$; GaN: $14.930 \times 10^{-17} \text{ Nps}^2 \text{ m}^{-1}$ and InN: $20.539 \times 10^{-17} \text{ Nps}^2 \text{ m}^{-1}$) due to their large thermal conductivity and acoustic coupling constants^{11,13}. This implies that the interaction between acoustical phonon and quanta of lattice vibration for *NdCuGe* is large in comparison to third group nitrides.

Conclusions

On the basis of above discussion, the following conclusions can be drawn:

- The theory for evaluation of higher order elastic constants is also valid for the hexagonal ternary rare-earth intermetallic compounds.
- For elastic properties, present results indicate that the ternary compound is brittle in nature and the obtained results for elastic constants thoroughly satisfy the established criterion of the mechanical

stability.

- The order of thermal relaxation time for *NdCuGe* intermetallic compound is found in picoseconds, which justifies their hexagonal structure. The re-establishment time for the equilibrium distribution of thermal phonons will be minimum for the wave propagation along $\theta = 90^\circ$ due to being smallest value of ' τ ' along this direction.
- The acoustic coupling constant of *NdCuGe* for longitudinal wave are found larger than third group nitrides. Hence the conversion of acoustic energy into thermal energy will be large for *NdCuGe* compound. This shows general suitability of chosen ternary material.
- The ultrasonic attenuation for longitudinal and shear wave are much greater than that of thermoelastic loss. This reveals that ultrasonic attenuation due to phonon-phonon interaction along Akhieser type of loss is governing factor for total attenuation and total attenuation is a governing factor for thermal conductivity and thermal energy density.
- The mechanical properties (yield strength, ductility, elastic properties) of *NdCuGe* at low temperature (50 K) are better than at room temperature, because at low temperature it has low ultrasonic attenuation.

Thus obtained results in the present work can be used for further investigations, general and industrial applications. Present theoretical approach is valid for temperature dependent ultrasonic characterization of intermetallic ternary compound *NdCuGe*. The ultrasonic behavior in *NdCuGe* as discussed above shows important microstructural characteristic features, which are well connected to thermoelectric properties of the material. These results, together with other well-known physical properties, may expand future prospects for the application and study of *NdCuGe*.

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A simple sonication-assisted exfoliation and characterization of few layered graphene nanosheets

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Reduced graphene oxide (rGO) is a radical candidate for energy related sector. In this paper, we report how few layers graphene that can be produced in large quantity with low defect ratio from exfoliation of GO by using a sonication energy. GO was prepared from graphite powder by modified Hummer's method. GO then further exfoliated to graphene oxide by using ultrasonic irradiation. The ultrasonication approach for the exfoliation of rGO nanosheet is relatively fast, cost-effective and efficient as compared to other methods. The characterization techniques such as UV and FT-IR analysis confirmed the reduction of GO to rGO. The structure and morphology of as-prepared rGO nanosheet were studied using a range of techniques such as XRD, Raman spectroscopy, SEM, and TEM. The experimental results suggest that the graphene sheets obtained by this simple exfoliation method after the heat reduction had an excellent exfoliation into a few layered graphene sheets.

Keywords: Ultrasonication, rGO, XRD, electron microscopy.

Introduction

Graphene is promising to be the most exciting material of the decade. It is proved that an ideal graphene sheet is highly ordered and shows several extraordinary physical, chemical, and mechanical properties. It is a thin layer of carbon atoms tightly packed together and it looks like a two 2D honeycomb lattice.

The preparation process of rGO involves three steps: Oxidation, exfoliation, and reduction. The most common modified Hummer's method was used to oxidize the graphite flakes. In this step, oxygen functional groups attached to the graphite lattices, thus increasing the interlayer between the sheets and permitting its exfoliation in individual GO platelets. Methods such as ultrasonication and magnetic stirring *etc.* can be used in graphene exfoliation.

Several groups demonstrated that the ultrasonication approach for the exfoliation of nanosheet bears remarkable physical and chemical properties and excellent performance than other methods. Moreover, it

is relatively fast, cost-effective and efficient as compared to other methods.

The process of liquid exfoliation is based on placing GO within a solvent which expands and helps to separate the weakly bonded layers of GO. Sonication of the solvent expanded mixture results in the production of single and multi-layered GO sheets. The resultant exfoliated GO can be conductive by exposing it to reducing agents

The last step is the reduction of this GO. The reduction process can be accomplished by several strategies, such as electrochemical reduction, thermal reduction, photocatalytic reduction, and chemical reduction. Literatures showed that thermally reduced GO bears remarkable physical and chemical properties and excellent performance than other compounds.

In this work, a facile ultrasonication route for the exfoliation of graphene oxide (GO) has been reported. As prepared sample was characterized using a range of techniques such as FTIR, UV, XRD, Raman spectroscopy, SEM, and TEM.

Materials and Method

Materials

Graphite flakes (aldrich), sulfuric acid (H_2SO_4), sodium nitrate ($NaNO_3$), potassium permanganate ($KMnO_4$), hydrogen peroxide (H_2O_2) were used in the process. All chemicals were used as received, without further purification. Double distilled water was used throughout the experiment.

Experimental procedure

Preparation of samples

Firstly, GO was prepared from the graphite powder by modified Hummer's method. Graphite powders were first oxidized by reacting them with concentrated H_2SO_4 (60 ml). The reaction vessel was placed in an ice bath, and $NaNO_3$ was added slowly. The reaction was allowed to go on for 24 hours to fully oxidize graphite into GO. The final products were then centrifuged, washed, and finally dried in a hot air oven.

In the second step, GO was suspended in a mixture of ethanol and water (1:1) and was exfoliated through ultrasonication for 1 hour. It was observed that the color of the suspension gradually changed into a yellowish brown solution. The final products were then centrifuged, washed, and finally dried in an oven.

The exfoliated GO was reduced to graphene nanosheet by thermal reduction method. The GO samples were heated up to $350^\circ C$ using a hot plate. The resultant product is the reduced GO or graphene.

Results and Discussion

The surface morphology and structure of the prepared graphene was characterized by TEM, SEM and XRD Raman analysis. UV and FTIR analysis further confirmed the reduction of GO to rGO.

FTIR analysis

The FTIR spectra of the prepared nanostructures are shown in Fig. 1. The characteristic peak at 1067 cm^{-1} decreased dramatically, confirms the reduction of GO. An absorption band that appears at 1578 cm^{-1} attributed to the skeletal vibration of the reduced graphite oxide. The peaks at 1633 cm^{-1} correspond to the vibration of carboxyl groups. In the FTIR spectrum of rGO, the characteristic absorption bands of $C=O$, $C-O$ and $O-H$

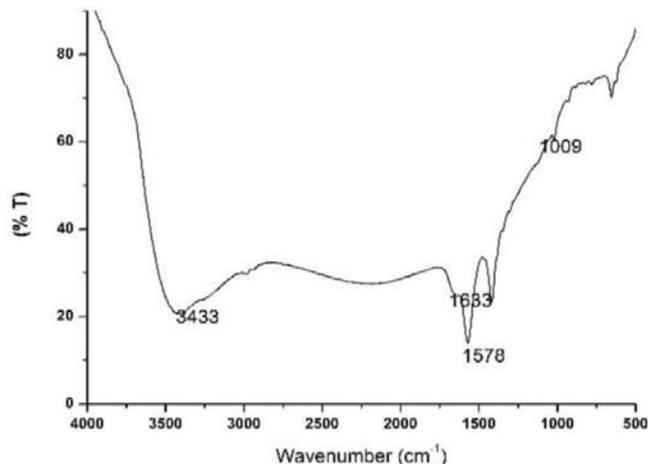


Fig. 1 FTIR analysis of rGO nanosheets

decreased dramatically, demonstrating that GO has been reduced.

UV-Vis analysis

Figure 2 shows the UV absorption spectrum for synthesized graphene sheets. The absorption peak around at 263 nm which shows the optical properties of the rGO sample. After the reduction of GO, the peak of the $\pi-\pi^*$ transition was shifted to 263 nm indicating that some groups on the GO surface were removed and the conjugated structure was restored.

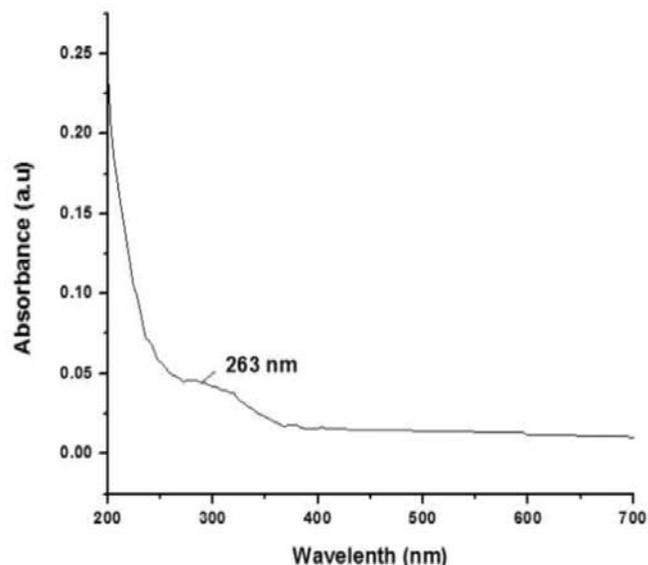


Fig. 2 UV analysis of rGO nanosheets

XRD analysis

The XRD pattern obtained for synthesized rGO nanoparticles shown in Fig. 3. A broad diffraction peak

appears at $2\theta = 23-28^\circ$ which can be indexed to the disordered rGO sheets. Moreover, the disappearance of the peak at 10° and appearance of the peak at 26° , ensures the reduction of GO into rGO by thermal reduction method.

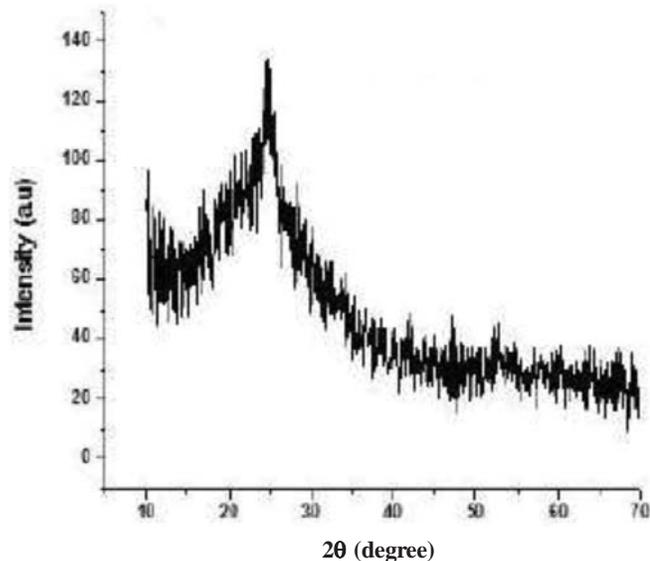


Fig. 3 XRD pattern of rGO nanosheets

Raman analysis

Figure 4 shows Raman spectra of graphene resulted from the sonication route exfoliation of graphene oxide. The presence of *D* and *G* bands also confirms the formation of graphene with lesser defects and crystalline structure. In Raman spectroscopy, *D* band indicates the extent of defects and the *G* band shows the graphitic

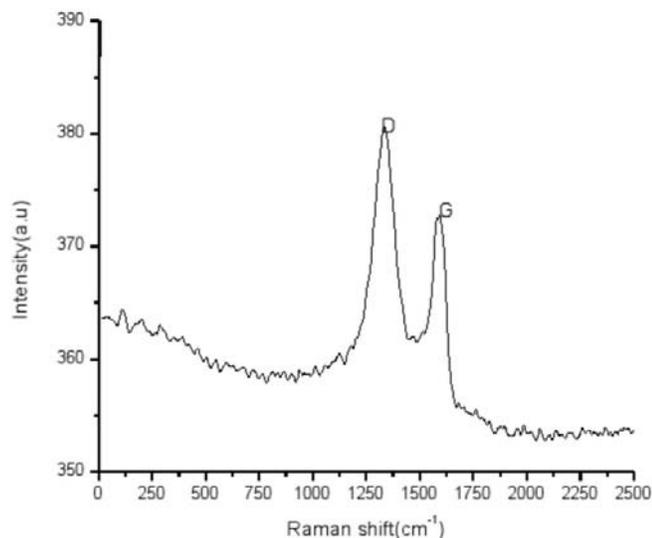


Fig. 4 Raman spectrum of rGO nanosheets

nature. If the *D* peak intensity is higher, the sample is having more defects in graphite network. If the *G* band is prominent, the sample is said to be crystalline. Here, the *D* and *G* bands are found at 1344 cm^{-1} and 1581 cm^{-1} , respectively. The *G* band around 1581 cm^{-1} , resulting from first-order scattering of the E_{2g} mode of the sp^2 carbon domains, is the evidence for the sp^2 carbon in the hexagonal graphene lattice.

SEM analysis

Figure 5 shows that the prepared sample contained well-exfoliated graphene sheets, including multilayers and some monolayers, with very large sheets. The sheets are almost transparent and have one or few layer 2D sheet structure with some obvious wrinkles.

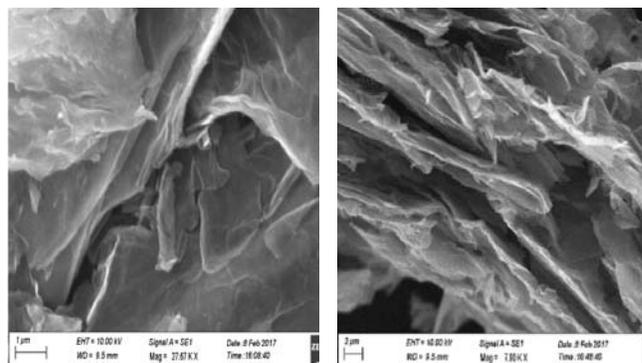


Fig. 5 SEM image of rGO nanosheets

TEM analysis

TEM analysis in Fig. 6 again confirms the morphology of rGO sample. The reduction processes of GO, the hydroxyl group of the GO reduced and a honeycomb-like structure has obtained.

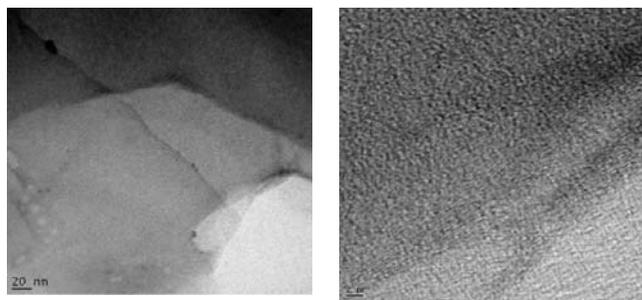


Fig. 6 TEM image of rGO nanosheets

Conclusions

The results of this study suggested that the graphene

powder obtained by this simple exfoliation method after the heat reduction had an excellent exfoliation into a few layered graphene sheets. UV and FTIR analysis confirmed the reduction of GO to rGO. From the XRD, a broad diffraction peak appears at $2\theta=23-28^\circ$ which can be indexed to the disordered rGO sheets. The Raman analysis further confirms the reduction of GO to rGO. The morphology of the samples was described by SEM and TEM. SEM observations demonstrated that graphene nanosheets are transparent and have one or few layers of 2D sheet structures with some wrinkles.

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Press Release

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Ph.D Thesis Summary

Development of a Long-Range Ultrasonic Imaging System in Air Using an Array Transmitter

(Awarded to Dr. Sahdev Kumar on March 23, 2017 by Aichi Institute of Technology, Toyota, Japan)

Ultrasonic sound waves are used for versatile applications in biomedical, industries, materials, security, device measurements and characterization for research and developments etc. owing to its simplicity, reliability, safety and non-destructive evaluation nature. The 3-D imaging and range-sensing applications have also been recently thrust areas and attracted considerable attention using ultrasonic technology. A conventional ultrasonic system has its limitation in the open air due to absorption. A high power ultrasonic source can be used for more distant objects imaging. A high power ultrasonic sound source was reported using spark-discharge method but it is not safe. In the process, this D. Eng. thesis work has been considered to develop an easy, simple and cost effective approach to generate high-power ultrasonic pulsed waves and demonstrated a 3-D imaging system upto 25 m that is two times higher than other conventional ultrasonic transmitters.

The ultrasonic array transmitter (UAT) consists of 12×12 elements with 10 mm inter-element spacing to generate directional high power ultrasonic pulses owing to the beams formation. Theoretical investigations are performed thorough simulations using MATLAB software programming to confirm apossibility of high power ultrasonic array transmitter and experimentally demonstrated for its 3-D range imaging application feasibility of an object without divergence control. The theoretical investigations are further extended to the isotropic and anisotropic divergence control to enhance the field-of-view with experimental demonstration in range

imaging. Developed ultrasonic imaging system consists of UAT (144 elements) and a receiver array (32 elements). A 40 kHz generated signal is pulse modulated using Field Programable Gate Array (FPGA) that controls each transmitting element independently. This system is evaluated by placing an object in air and receiving the echo of the transmitted pulse. Delay-and-sum (DAS) method is applied on the reflected received signal to find the image of the object in a 21×21 pixels scale with $105^\circ \times 105^\circ$ view angle. Whole system is controlled by personal computer and out put of the hardware using simulink shows signal intensity and range of the object through its colour match on the colour bar. This sophisticated computer-controlled system is capable of driving the multi-element probes, receiving and digitizing the returning echoes for plotting echo information in various standard formats. Unlike conventional flaw detectors, phased array systems can sweep a sound beam through a range of refracted angles along a linear path or dynamically focus at a number of different depths increasing the flexibility and inspection use. A compact and high resolution range imaging system using UAT can be expected by MEMS technology for its optimized system performance in various applications with higher accuracy and reliability. This D. Eng. research work resulted in four International Journal research papers and twelve international and national conferences papers presented in Europe, South Africa, Thailand, India and Japan with financial support by JSPS and Rotary Yoneyama Memorial Foundation.

National Symposium on Advances in Ultrasonics and Materials Research

XXII National Symposium on Advances in Ultrasonics and Materials Research was organized 8th to 10th November 2017 at Department of Physics and Astronomical Science, Central University of Himachal Pradesh (CUHP) in association with Ultrasonics Society of India (USI), NPL New Delhi. The symposium was held at **Chinmaya Organization for Rural Development (CORD) Trust Auditorium in Tapovan, Dharamshala (H.P.)**. Dr. B. C. Chauhan, (Head-DPAS & Dean-SOPMS); Dr. O. S. K. S. Sastri (Associate Professor), Dr. Padmnabh Rai (UGC-Assistant Professor), Dr. Jagdish Kumar (Assistant Professor) and Dr. Rajesh Kumar Singh (UGC-Assistant Professor) from Department of Physics & Astronomical Science (DPAS) under School of Physical & Material Sciences (SOPMS) in CUHP, Dharamshala (HP) were the Chairman, Co-chairman, Convener, Academic Secretary and Organising Secretary for the conference, respectively.

The main focus of the conference was around following areas :

Ultrasonics and its Applications in Material Science; Ultrasonic NDT; Underwater Acoustics; Biomedical Ultrasound; Sonochemistry; Physical Acoustics; Nanomaterials and their Applications; Potential Applications of CVD Techniques; Nano scale Electronics and Photonics; Ultrasonic transducer materials; Plasmonics and Metamaterials; Energy Harvesting Materials; Modern Superconducting Materials; Sensors and Applications; Materials for Optical Applications; Dirac Materials; Modelling and Simulations of Materials; Multifunctional Materials; Carbon based Smart Materials; Ancient Indian Science & Technology.

The details of registered participants were as follows:

- No. of Invited Speakers: 17
- No. of Registered participants from Universities /Scientists from National Labs/Persons from other Institutes Participated: 41

- No. of Registered person from corporate sector: 2
- No. of Registered PG Students from CUHP: 27
- No. of research scholar Registered from CUHP: 10
- No. of Registered faculty members from CUHP: 23
- No. of Registered other staff committee members from C.U.H.P.: 7

The inauguration of the symposium was done with **Saraswati Poojan** in the presence of many dignitaries including **Prof. H. R. Sharma**, Pro-Vice Chancellor CUHP; **Prof. Vikram Kumar**, President Ultrasonics Society of India and Professor IIT Delhi; **Prof. Raja Ram Yadav**, Vice Chancellor VBS Purvanchal University, Jaunpur; Prof. B.C. Chauhan, Dean of School of Physical and Material Sciences, CUHP and Prof. O.S.K.S. Sastri from Department of Physics and Astronomical Sciences CUHP. Prof. OSKS Sastri welcomed the participants to the symposium emphasizing its importance taking cues from ancient Indian science. Prof. B.C. Chauhan delivered the inaugural address wherein he elaborated how the university is gaining high standard in providing research and higher education in various fields including physical and material sciences. Prof. Vikram Kumar president of USI introduced the participants about USI and its objectives.

Prof. Raja Ram Yadav, the Chief Guest, informed the gathering about his special association with CUHP. He also linked ancient Indian science with acoustics and ultrasonics. Dr. Yudhisther Kumar Yadav, General Secretary USI, announced the USI awards. Dr. T K Saksena Award 2017 for the best thesis was presented to Dr. Punit Kumar Dhawan from Allahabad University and Dr. S Parthasarathy Award was presented to Dr. Sahdev Kumar and Dr. Ganeswar Nath for their papers published in the Journal of Pure and Applied Ultrasonics for the year 2016. The inaugural session was followed by high tea.

The first session of the symposium begun with *plenary talk* by Prof. Vikram Kumar from IIT Delhi, who discussed the Research Challenges for Photovoltaics. In this talk he spoke about the recent thrust by the Indian Government on solar energy, of which the photovoltaic research and development is an important component. Prof. Vikram Kumar pointed out that while the PV market continues to be dominated by the silicon crystalline solar cells which are largely imported, there is a need to improve the silicon cells as they have some limitations. He mentioned about his experience as the chair for PV effort at MNRE as well as DST for last few years, during which he has placed special emphasis on developing silicon technologies in Indian research institutes. In his talk, he reviewed the current status of PV research particularly from Indian perspective. He also talked about silicon solar cell research taking place in Indian laboratories and recent developments in nanowire solar cells.

After this, Dr. Yudhisther Kumar Yadav from NPL, New Delhi presented his invited talk on *Ultrasonic Power Measurement and its Applications in Biomedical Industry*. The next invited talk was by Dr. Mahavir Singh from NPL New Delhi delivered his talk on *Reliable Measurements of Sound Absorption Coefficient in the Reverberation Chamber*. The first session was chaired by Prof. Raja Ram Yadav. The first session was followed by a lunch break.

The second session chaired by Prof. B.C. Chauhan which started with the invited talk by Prof. P.K. Mukhopadhyay of S.N. Bose Centre for Basic Sciences, Kolkata on *Elastic Moduli of Ni-Fe-Al Ferromagnetic Shape Memory Alloy Studied by Resonant Ultrasound Spectroscopy*. It was followed by another invited talk by Dr. S. K. Kushwaha on *Laser MBE Growth and Characterization of GaN Nanostructures and Epitaxial Layers for various Applications*. After this session, an oral session on presentations by five participants was held, which was chaired by Dr. Dalip Singh Verma. At the end of the day the poster session was organised in which fourteen researchers presented their research work. The presentations were judged by Dr. Y. K. Yadav and Dr. Ayan Chatterjee.

The second day of the symposium started with the plenary talk by Prof. Raja Ram Yadav on topic *Application of Ultrasonics in Nanotechnology and Biology*. Prof. Raja Ram Yadav highlighted that ultrasonic techniques have become very important not

only to characterize the advanced materials but also act as a cost effective replacement to highly expensive transmission electron spectroscopic method up to some extent. "For any characterization scheme, study of ultrasonic propagation behavior in materials under different physical/microstructural conditions has become a prerequisite" he added. He presented pioneering results on ZnO nanoparticles based ethylene glycol nanofluids which are important materials for biosensing and coolant technology. He presented how the size of the nanoparticles and their distribution were determined using the ultrasonic spectroscopy method. He also presented the theoretical modelling on temperature dependent anomalously enhanced thermal conductivity of the same.

The invited talks were presented by Prof. Rita Paikaray from Ravenshaw University, Cuttack on topic *Ultrasonic science in utilization of waste material*; Prof. P.S. Saxena from BHU on *Applications of nano-materials in biology*; Dr. P. K. Tyagi of Delhi Technological University on *CVD growth of carbon based modern materials*; Prof. Prabhakar Singh of IIT BHU on *Solid Oxide fuel cells*. This session was chaired by Prof. Anchal Srivastav of IIT BHU.

The next session of the day and was chaired by Prof. O.S.K.S. Sastri from CUHP. In this session the invited talks were by Prof. B. C. Chauhan on *Indian Tradition of Science* and Dr. V.R. Singh of NPL on topic *IOT and smart ultrasonic sensors for U-health care*.

The last session of the day after tea was chaired by Dr. Y. K. Yadav. There was one invited talk delivered by Dr. S K Jain on *Force Sensing and Actuation using Piezoelectric Techniques* and six oral presentations in this session. The presentation by Dr. S.K. Jain was relevant for applications such as robotics, surgery, industry and research. After this, the poster session II was held. In this session almost 14 researchers presented their research work in form of posters. The judges for poster session were Dr. Surender Verma and Dr. P. K. Tyagi.

On day 3 of NSU-2017, the first session started with invited talk by Prof. Anchal Srivastava from BHU Varanasi who presented his talk on *Nanotechnology: Black is Meaningful (Carbon Nanotube and Graphene)*. The second invited talk in this session was presented by Dr. S.K. Dubey of IIT Delhi on *Optical sensors with healthcare applications*. This session was



chaired by Prof. Vikram Kumar. The second session started after tea break and was chaired by Dr. V.R. Singh. In this session two invited talks were presented. The first talk was by Dr. Devraj Singh of Amity School of Engineering, Delhi on topic *Elastic, Ultrasonic and Thermophysical Properties of Materials for Advanced applications* and the second talk by Prof. V. A. Tabhane from Pune University.

Apart from all these activities, a picture exhibition on Ancient Indian Science was organised in the conference under the guidance of Prof. B. C. Chauhan.

The valedictory function of NSU-2017 was organized after lunch on 10th November 2017. Vice Chancellor of CUHP Prof. Kuldeep Chand Agnihotri was the Chief Guest for the session. The function began with Saraswati Vandana and Poojan. Prof. Agnihotri presented his gratitude to participants for their participation in NSU-2017 and making it a grand success. He also highlighted the leading role played by ancient Indian scientists in development of human beings. He emphasized the need for bridging the gap between rich ancient scientific ideas presented in our Vedas and modern technology.

Finally, different awards were presented to the participants by the Chief Guest Prof. K. C. Agnihotri for following categories:

- Nishant Kumar, Kiran Soni and R. Aggarwal from Thapar University Patiala got the Dr. M Pancholy Memorial Award for the best oral paper presented at National Symposium on Ultrasonics
- Alok Kumar Verma and R.R. Yadav from University of Allahabad got the best oral paper in field of ultrasonic in material science.
- Amireddy Kiran Kumar, Prabhu Rajagopal and K. Balasubramaniam from Centre of NDE, Dept. of Mech. Engg. , IIT Madras got the best poster paper in Ultrasonic Field.
- Vijay Kumar Singh, R.S. Tiwari, Anchal Srivastva from Institute of Science, BHU got the best poster in material science.
- Chinmayee Tripathi, Devraj Singh and Rita Paikare from Ravenshaw University, Cuttack got second best poster in Ultrasonics.
- Nitika Devi, Rajesh K. Singh, A. K. Jaiswal from CUHP got second best poster in material science.

At the end of the conference, Dr. Bhag Chand Chauhan presented the vote of thanks and his appreciations to the organising team.

— **Dr. Padmanabh Rai**
Convener - NSU-2017

Central University, Himachal Pradesh, Dharamshala

AN OBITUARY



Dr. Baldev Raj

Dr. Baldev Raj, a Distinguished Scientist, Padma Shree Awardee, renowned administrator of nuclear power science and technologies of our country and the Director of the National Institute of Advanced Studies (NIAS), Bengaluru, passed away on January 6, 2018, aged 70 at Pune. Raj had assumed leadership of the NIAS in 2014. Previously, he had served as the President of Research at P.S.G. Institutions (2011-2014), Coimbatore, and as the Director of the Indira Gandhi Centre for Atomic Research (2004-2011), Kalpakkam. Born on April 9, 1947, he had a distinguished degree in metallurgy from NIT Raipur, completed his Ph.D. in Engineering from the Indian Institute of Science during 1989. Dr. Raj had his initial training in nuclear technology from the Bhabha Atomic Research Centre (BARC), Trombay.

Being a Metallurgist, he pioneered into the field of Non-destructive Testing and Evaluation (NDT&E) of materials and components under the able guidance of exemplary personality and former Director of IGCAR Dr. Placid Rodriguez during 1980's at Kalpakkam and flourished in his endeavor. And today his name is well known throughout the world among NDT community and companies. Dr. Raj was the President of the Ultrasonic Society of India (USI) from 1999 - 2004. Under his presidential ship our USI achieved astounding membership numbers. Likewise, he promoted the Indian society of Non-destructive Testing (ISNT) to greater heights bringing it international recognition. Used his abilities in NDT studies and management skills to promote the on-going research and technological programmes of the Prototype Fast Breeder Reactor (PFBR). This led to the better understanding the properties of materials used in nuclear power plants and to efficiently manage the trouble free operation of PFBR and also to extend its service life. A totally indigenous 500-MWe PFBR unit at Kalpakkam named "BHAVINI" is set to go critical soon.

Also, Dr. Raj had a deep interest in Indian Archeology, wherein he employed several metallurgical and NDT techniques to better the understanding of their constituents, ancient metallurgy, casting techniques, etc. for their long term preservation and also to protect them from smugglers. To name a few: Thanjavur Chola Bronzes, Hampi Musical Stone Pillars, Delhi Iron Pillar, *etc.*

He authored more than 800 publications in refereed journals & book volumes and 60 books. He had also contributed technical manuscripts to several special journal volumes, encyclopedia and handbooks. He was a combined owner of 21 patents as well. He was recognized by way of awards, honours, plenary and keynote talks, editorial positions and assignments in esteemed national and international forums in more than 30 countries. He was editor-in-chief of three series of books. He was conferred with Distinguished Alumnus Award of Indian Institute of Science, Distinguished Materials Scientist Award of Materials Research Society of India, National Metallurgist Award of Ministry of Steel, Government of India, Presidential honour Padma Shree, Indian Nuclear Society's Life Time Achievement Award (2011), Homi J Bhabha Gold Medal (received from the Prime Minister of India during 99th Indian Science Congress 2012) and Nayudamma Memorial Award (2012).

Apart from his research, Dr. Raj worked closely with the National Institution for Transforming India (NITI Aayog), to develop science action plans for up to 15 years in the future, to advise the Department of Science and Technology on clean energy, and to carry forth consultation with the government on the extraction of rare-earth metals. In 2017, Prime Minister Narendra Modi appointed him as Chairperson of the board of governors of the Academy of Scientific and Innovative Research for a period of five years. According to a statement issued by the NIAS upon his demise, "He led the institute to new heights in terms of multi-disciplinary pursuits, and brought it closer to the government's decision-making processes".

We the USI Community sincerely express our heartfelt condolences to the family and friends and colleagues of Dr. Baldev Raj.

Dr. P. Palanichamy
Member, Editorial Board, JPAU
Formerly Scientist, Nondestructive Testing Division
IGCAR, Kalpakkam

Journal of Pure and Applied Ultrasonics

(INDEXED IN: Indian Citation Index, Google Scholar, i-Scholar, UGC List)

INFORMATION FOR AUTHORS

1. Type of Contribution

JOURNAL OF PURE AND APPLIED ULTRASONICS welcomes contributions on all aspects of ultrasonics including ultrasonic studies in medical ultrasonics, NDT, underwater, transducers, materials & devices and any other related topic. Contributions should fall into one of the following classes.

Paper - These should be on original research work contributing to scientific developments. They should be written with a wide readership in mind and should emphasize the significance of the work.

Reviews and Articles - Includes critical reviews and survey articles.

Research and Technical notes - These should be short descriptions of new techniques, applications, instruments and components.

Letters to the editor - Letters will be published on points arising out of published articles and papers and on questions of opinion.

Miscellaneous - Miscellaneous contributions such as studies, interpretive and tutorial articles, conference reports and news items are also accepted. Recommended contribution lengths are: Papers 2000-4000 words. Reviews and Surveys 2000-5000 words; Conference Reports 500-1500 words; News Items, Research and Technical Notes up to 1000 words.

2. Manuscripts

Manuscripts should be typed on one side of the paper in double spacing with 25 mm margin on all sides of A4 size paper. A soft copy of the manuscript in MS

WORD for text and MS EXCEL for illustrations and a PDF file thereof may be sent by e-mail or CD/DVD. Colour images should be formatted as JPEG files. Figures submitted in colour would be published in colour. Colour should be avoided unless it is required in order to convey a message or serve a purpose in the image.

Title - Titles should be short and indicate the nature of the contribution.

Abstract - An abstract of 100-200 words should be provided on the title page of paper and review article. This should indicate the full scope of the contribution and include the principal conclusions.

Mathematics - Mathematical expressions should be arranged to occupy the minimum number of lines consistent with clarity e.g., $(x^2+y^2)/(x-y)^{1/2}$.

Illustration - The line illustrations along with captions should be clearly drawn with black Indian ink. Figures in Excel are preferred.

References - References should be referred to in the text by number only. The reference number should be given as superscript. The corresponding reference shall contain the following information in order; names and initials of author (s)(bold), title of the work, journal or book title (italic), volume number (bold), year of publication in brackets, page number, e.g., **Kumar S. and Furuhashi H.**, Anisotropic divergence controlled ultrasonic transmitter array for three dimensional range imaging, *J. Pure Appl. Ultrason.*, **38** (2016) 49-57.

Units and Abbreviations - Authors should use SI units wherever possible.