ON THE BEHAVIOR OF THERMO ACOUSTIC PARAMETERS IN THERMAL BARRIER COATING MATERIALS

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Abstract

The thermo acoustic parameters of Thermal Barrier Coating Materials are estimated in terms of the thermal expansion coefficient (α) at 1273 K on the assumption that the Moelwyn-Hughes parameter (C_1) is the dominant factor. The Moelwyn-Hughes parameter has been employed in various established relations and evaluated lattice Gruneisen parameter (Γ), non-linear Beyer's parameter (B/A), the free available volume (V_a/V), the repulsive exponent of intermolecular potential (n), the reduced molar volume ($\tilde{V}$), the reduced compressibility (β), isochoric acoustical parameter (Δ), the Anderson-Gruneisen parameter (δ), the Sharma's parameter(S_0) and other parameters. The relationship between the Γ_{ith} , Γ_{ich} , and Γ_{iba} has been studied and the magnitudes are interpreted in terms of the characteristic behavior of material. The parameter Y is found to be close to 0.10 which may infer that the normal modes of vibrations contributing to heat capacities are almost negligible. Sharma's parameter has been found to be constant i.e., 1.10. The present study gives an opportunity to understand the significance of fractional free volume and the S_0 parameter in describing the anharmonic and non-linear properties of these materials.

***Keywords**: Thermal Barrier Coating Materials, Moelwyn-Hughes parameter, Thermo acoustic parameters*

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1. INTRODUCTION

Rare earths are a series of minerals with special properties that make them essential for applications including miniaturized electronics, computer hard disks, display panels, missile guidance, pollution controlling catalysts, H_2-storage and other advanced materials. The use of thermal barrier coatings (TBCs) has the potential to extend the working temperature and the life of a gas turbine by providing a layer of thermal insulation between the metallic substrate and the hot gas [1, 2].

Rare earth oxides have very high melting points, low thermal conductivities and large thermal expansion coefficients, and the addition of any rare earth oxide into a ceramic material usually results in the reduction of thermal conductivity and the increase of thermal expansion coefficient which are two very important properties for a TBC material. In view of their potential properties and applications of rare earths in TBC materials, thermo acoustic properties have been investigated.

In the present work thermo acoustical parameters viz, the isothermal, isobaric and isochoric Gruneisen parameters, Beyer's nonlinearity parameter, the free available volume, the repulsive exponent, the reduced bulk modulus compressibility, the Anderson-Gruneisen parameter and thermo acoustical parameters have been evaluated in TBC materials at 1273K.

2. THEORY

The necessary data on the volume expansivity (α) at 1273 K for the Thermal Barrier Coating materials has been taken from the literature [3]. Several authors have reported the estimation of thermo acoustic parameters in the literature [4-10, 18]. As various authors have reported the details of the said approach, only the results of the work are given in Table 1(a) and Table 1(b).

3. RESULTS AND DISCUSSION

The necessary experimental (α) values for the TBC materials have been taken from the literature [3]. Tables 1(a) and 1(b) give the calculated values of different thermoacoustical parameters α, C_1,V_a/V, B/A, $\tilde{V}$, β, r, S_0, S^* etc., using the formulae given by Reddy et al. [5,6] at temperature 1273 K. The present treatment has the great advantage to describe thermo acoustical parameters of TBC materials employing only expansivity data. This study gives an opportunity to test the relation between C_1, B/A, V_a/V and other parameters. The validity of these equations is clearly tested in the present study using experimental data.

Moelwyn-Hughes parameter C_1 shows the increase trend as (α) value decrease which shows the variation of volume expansivity with temperature. Bayer's non-linearity parameter B/A is strongly structure dependent quantity and characterizes the lattice behavior of materials. It shows decrease trend as (α) values increases. The decrease of this parameter with (α) shows the increase in intermolecular modes of vibrations and anharmonicity in these materials.

This shows the associating nature and weak intermolecular forces in these materials. Reduced volume ($\tilde{V}$) and free available volume (f) are identical in nature. Reduced volume ($\tilde{V}$) shows a linear increase with (α) increase. If the available volume has a small value then fractional free volume would also have a small value. This shows the variation in size of these materials. The increase in available volume with raising temperature is quite natural phenomenon and it is attributed due to increase in intermolecular attraction at higher temperatures.

The high value of repulsive exponent (n) shows the bulk nature of molecule. Repulsive exponent is found to show a decrease with (α). It is pertain to mention that the decrease in n with (α) shows the dissociating nature of molecules and the increase in n shows associating nature of molecules. It is also interesting to highlight that the parameter isochoric thermo acoustic parameter (Δ) have on the average, a constant value of 0.36 and Y=0.11 for all the above materials studied. In the present work the isochoric temperature coefficient of volume expansivity shows negative values. The values of isochoric temperature coefficient of volume expansivity is reported in Table 1(b).

Sharma[11] introduced three dimensionless anharmonic parameters for the liquid state, namely, isobaric (Γ_{iba}), isothermal (Γ_{ith}), and the isochoric (Γ_{ich}), microscopic Gruneisen parameters, which may be shown to be related as

$$\Gamma_{ith} = \Gamma_{ich} + \Gamma_{iba}.$$

It is related to internal pressure which measures the instantaneous volume derivative of the intermolecular cohesive energy associated with an isothermal expansion of the liquid[11]. Γ_{ich} is negative quantity for polymers and semiconductors and positive for liquids [6, 8]. Γ_{ich} value for a material decides whether $\Gamma_{iba} \geq \Gamma_{ith}$. It is quite known that $\Gamma_{iba} < \Gamma_{ith}$ in the case of liquids and $\Gamma_{iba} > \Gamma_{ith}$ for Thermal Barrier Coating materials.

The estimated Γ_{ich} and θ are found to be negative. The more the thermal expansion coefficient (α), the less is the negative value for θ. The reduced compressibility β varies from 2.81 to 2.83 in the case of TBC materials. Several investigators [8,10,12-17] reported that the constant S_0 is (1.11$\pm$0.01) for any system existing either in liquid or in a solid state. The Sharma constant S_0 in TBC materials is found to be of the order of 1.10. The other constant S^* has been found to be around 1.01 and is seen to be fairly constant for all the materials studied.

Molecular constant 'r' measures the molecular cohesion. If 'r' is low then the state of the material causes a molecular dissociative effective due to increasingly loose packing of the molecules resulting in a very weak intermolecular cohesion [5]. The molecular constant 'r' in the present study is of the order 1.56 to 1.57 and which is equal to the dimension reciprocal of volume. The reduction in the value of 'r' shows an increasing in molecular order and the increase in 'r' with mass concentration shows decrease in molecular order.

Table 1(a): Thermo acoustic properties of TBC materials at 1273 K

Material	$\alpha \times 10^{-6}$	C_1	Γ	(B/A)	n	(V_a/V)	$\tilde{V}$	β	X	Δ
4.52YSZ	11.0	75.761	37.382	74.761	215.283	0.0260	1.0138	2.8393	-0.000568	0.362
$La_2 Zr_2 O_7$	9.1	90.669	44.836	89.669	260.007	0.0218	1.0114	2.8174	-0.000570	0.363
$La_{1.4} Nd_{0.6} Zr_2O_7$	8.7	94.637	46.820	93.637	271.911	0.0209	1.0109	2.8133	-0.000570	0.363
$Nd_2 Zr_2O_7$	9.6	86.173	42.589	85.173	246.521	0.0229	1.0121	2.8244	-0.000569	0.362
$La_{1.4} Gd_{0.6} Zr_2O_7$	9.3	88.813	43.908	87.813	254.439	0.0222	1.0117	2.8210	-0.000570	0.362
$Gd_2 Zr_2 O_7$	10.4	79.880	39.442	78.880	227.642	0.0247	1.0131	2.8333	-0.000569	0.362
$La_{1.4} Eu_{0.6} Zr_2 O_7$	9.2	89.731	44.367	88.731	257.193	0.0220	1.0116	2.8199	-0.000570	0.363
$La Eu Zr_2 O_7$	10.6	78.456	38.730	77.456	223.368	0.0251	1.0133	2.8356	-0.000569	0.362
$Eu_2 Zr_2 O_7$	9.5	87.035	43.019	86.035	249.105	0.0227	1.0120	2.8233	-0.000569	0.362
$La_{1.7} Dy_{0.3} Zr_2O_7$	8.9	92.608	45.806	91.608	265.825	0.0213	1.0112	2.8166	-0.000570	0.363
$La_2 Zr_{1.8} Ta_{0.2} O_7$	8.7	94.637	46.820	93.637	271.911	0.0209	1.0109	2.8143	-0.000570	0.363
$La_{1.92} Ca_{0.08} Zr_2O_7$	8.8	93.611	46.307	92.611	268.834	0.0211	1.0111	2.8155	-0.000570	0.363

Table 1(b): Thermo acoustic properties of TBC materials at 1273

Material	$\alpha \times 10^{-6}$	Γ_{ith}	Γ_{ich}	Γ_{iba}	δ	θ	Y	r	S_0	S^*
4.52YSZ	11.0	37.380	-24.85	62.235	124.47	-48.70	0.1102	1.5674	1.1063	1.0186
$La_2 Zr_2 O_7$	9.1	44.834	-30.34	75.180	150.36	-59.69	0.1104	1.5701	1.1061	1.0154
$La_{1.4} Nd_{0.6} Zr_2O_7$	8.7	46.818	-31.80	78.623	157.24	-62.60	0.1104	1.5705	1.1059	1.0147
$Nd_2 Zr_2O_7$	9.6	42.586	-28.67	71.263	142.52	-56.35	0.1103	1.5690	1.1057	1.0163
$La_{1.4} Gd_{0.6} Zr_2O_7$	9.3	43.906	-29.65	73.556	147.11	-58.29	0.1103	1.5693	1.1055	1.0157
$Gd_2 Zr_2 O_7$	10.4	39.440	-26.36	65.804	131.60	-51.72	0.1103	1.5680	1.1059	1.0176
$La_{1.4} Eu_{0.6} Zr_2 O_7$	9.2	44.365	-29.98	74.353	148.70	-58.97	0.1104	1.5696	1.1057	1.0156
$La\ Eu\ Zr_2 O_7$	10.6	38.728	-25.83	64.567	129.13	-50.67	0.1102	1.5676	1.1058	1.0180
$Eu_2 Zr_2 O_7$	9.5	43.017	-28.99	72.012	144.02	-56.98	0.1103	1.5691	1.1056	1.0161
$La_{1.7} Dy_{0.3} Zr_2 O_7$	8.9	45.804	-31.04	76.850	153.70	-61.09	0.1104	1.5700	1.1056	1.0151
$La_2 Zr_{1.8} Ta_{0.2} O_7$	8.7	46.818	-31.78	78.605	157.21	-62.57	0.1104	1.5703	1.1056	1.0147
$La_{1.92} Ca_{0.08} Zr_2 O_7$	8.8	46.305	-31.41	77.720	155.44	-61.82	0.1104	1.5701	1.1056	1.0149

4. CONCLUSION

In this paper we evaluated the thermo acoustic parameters of Thermal Barrier Coating Materials by employing only thermal expansivity data. It is known from the study that the elements with small (α) yield higher thermo acoustic parameters viz. C_1, Γ_{ith}, Γ_{iba}, δ and vice-versa. Reduced volume ($\tilde{V}$) shows a linear increase with (α) increase. The parameter isochoric thermo acoustic parameter (Δ) have on the average, a constant value of 0.36 and Y=0.11 for all the above materials studied. In the present work the isochoric temperature coefficient of volume expansivity shows negative values. The reduced compressibility β varies from 2.81 to 2.83 in the case of TBC materials. The Sharma constant S_0 in TBC materials is found to be of the order of 1.10. The other constant S^* has been found to be around 1.01 and is seen to be fairly constant for all the materials studied.

ACKNOWLEDGEMENTS

Authors are thankful to the Department of Physics for providing laboratory facilities. The authors are thankful for facilities and grants given under UGC-SAP for Department Research Support (DRS) and Department of Science & Technology (DST) New Delhi for Fund for Improvement of Science & Technology (FIST).

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