East European Journal of Physics. 4. 227-233 (2024)
DOI:10.26565/2312-4334-2024-4-22 ISSN 2312-4334

ELASTIC PROPERTIES OF C-TYPE LANTHANIDE SESQUIOXIDES

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Received August 8, 2024; revised November 5, 2024; accepted November 7, 2024

In this study, we have presented the solid-state theory of plasma oscillations to investigate the anisotropic elastic properties such as three independent static elastic stiffness constants (C_{ij}: C_{11}, C_{12} & C_{44}) of C-type Ln_2O_3 lanthanide solids. The calculated values of the static elastic stiffness constants of Ln_2O_3 are in excellent agreement with the theoretical results obtained by using ab-initio techniques. The values of elastic stiffness constants (C_{ij}) exhibit a linear relationship when plotted against their plasma energies and lie on a straight line. To further examine the validity of the present estimations on elastic moduli and other parameters of these materials. The mechanical moduli such as bulk modulus (B), shear modulus (G), Young modulus (E), Poisson's ratio (ν), shear wave constant (C_s), Cauchy pressure (C^*), Lame's coefficient (λ and μ), Kleinman parameter (ξ) Grunesien parameter (γ), Zener anisotropic constant (Z) and Pugh ratio (G/B) of lanthanide solids have also been investigated. For the lanthanide sesquioxide materials, the values of static elastic stiffness constants C_{ij} and elastic moduli were presented for the first time. Unfortunately, in the current study, for many parameters of these materials, experimental results were not found for a comparison with our theoretical predictions. Our estimations agree well with the available experimental data and other theoretical reports.
Keywords: *Elastic properties; Plasmon energy; Ln_2O_3*
PACS: 71.20.-b; 71.20.Eh; 71.20.Nr; 62.20.de

1. INTRODUCTION

Sesquioxide of lanthanide metals are very important technological inorganic materials due to their outstanding thermo-physical and thermo-chemical properties. Lanthanides sesquioxide in cubic structure with general formula Ln_2O_3 (Ln = La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) are the subject of theoretical and chemical research extensively due to their interesting structural, semiconducting, elastic, mechanical, thermal properties and wide industrial applications such as industrial catalysis, Biomedical applications, Solis-State lighting, permanent magnets, hydrogen storage and nuclear energy fuels, lasers, optical display, Solid state fuel cells and neutron absorber for nuclear control etc. [1-7]. Lanthanide sesquioxide metals are n-type wide band gap semiconductors with low carrier mobility and very high refractive index [8, 9]. It is well known for below the temperature 2000°C, the structure of sesquioxide crystals exists in three phases; (i) A-type, Hexagonal in space P3mI (ii) B-type, monoclinic in space group (C2/m) (iii) C-type, Cubic in space group (Ia3) [10] and above the temperature, these materials appearance in X-phase and H-phase have been reported [11]. The unit cell of cubic structured Ln_2O_3 can be built up of 8-unit cells of fluorite structure (Fm3m) by removing 25% O-atom and ordering the remaining oxygen in remaining way. In particular, Ln-atoms are surrounded by 6 O-atoms is surrounded by 4-lanthanide atoms [12]. Since, in the sesquioxide form of lanthanide compounds, these atoms are in trivalent oxidation state and show the three electrons in conduction band partially filled p-orbital of oxygen atoms "4f" electrons are strongly localized on the rare earth atoms [13]. Hirosaki et al. [14] have focused the first principles pseudo potential calculation of the equilibrium crystal lattice dimension for most lanthanide oxides Ln_2O_3 using Vienna Ab-initio simulation package (VASP). Prokofiev et al [15] have studied the optical band gap on single crystals of the Ln_2O_3 series. The electronic and optical properties of Ln_2O_3 series analyzed by Singh et al [16] and employing the FPLAP method with in Local Spin Density Approximation [LSDA] and Coulomb Corrected Local Density Approximation [LSDA+U] as implemented in the WIEN2K code. The equilibrium volume and bulk modulus of hexagonal and cubic structured RE_2O_3 investigated within the CSM approach [12].

Recently, Pathak et al [17] have been calculated the structural, elastic and mechanical properties of Ln_2O_3 via Ab-initio study. Important details of the electronic, optical, mechanical and structural properties of Re_2O_3 and Re_2S_3 crystals are revealed by many workers [18-24]. The density functional theory is to be limited on optical, electronic and structural properties of rare earth sesquioxides. For such materials the theoretical and experimental details of elastic properties of lanthanide sesquioxides are very rarer so far. Shafiq and coworker [25] have been investigates the elastic properties of lanthanide mono-oxides using DFT calculations. Rare earth oxides have increasingly turned into the focus of first principle studies due to their importance in fundamental research and practical applications [14, 15, 26]. To the best in

Cite as: P. Yadav, D.S. Yadav, D. Singh, P. Singh, A.S. Verma, East Eur. J. Phys. 4, 227 (2024), https://doi.org/10.26565/2312-4334-2024-4-22

our current knowledge, anisotropic elastic properties of lanthanide sesquioxide series have not been investigated experimentally due to the various difficulties to found accurate results of such materials. Pathak et al [17] have been lead to fill-up this gap by the calculation of elastic properties for only six Ln_2O_3 (Ln = Pm, Sm, Eu, Gd, Tb, Dy) employing ab-initio study. In many cases their results are slightly differ and, in few cases, no satisfactory results are thus found. It is very difficult problem to associate with experimental method and their high cost, as well as difficulties to obtained accuracy in results of their physical properties, due to this, researchers turned to studying the elastic, optical, thermal and structural properties of solids state materials through different theoretical techniques. Due to a large process and the complicated computational methods employing a series of approximations, such a process has always been complicated [27-31]. In the recent past few years, on the basis of semi-empirical models the theoretical calculations have become an essential part of the material research. Since empirical formulae do not give highly accurate results for each material in many cases but they can still be very useful. An empirical concept such as valence electron concentrations, empirical radii, iconicity and Plasmon energy are then useful [32-34]. Recently, Yadav and coworkers [35-40] have been studied the structural, optical, electronic, mechanical and thermal properties of binary, ternary chalcopyrite semiconductors and rare earth chalcogenides employing the plasma energy of solids as a key parameter, which depends on the number of valence electrons and it is changed when a metal forms the compound. Although various theoretical predictions for different types of the material using plasma oscillation theory of solids are obtained in literature [31-34], to the best of my knowledge, there are no theoretical investigations on structural, optical, mechanical and elastic properties of C-type lanthanide sesquioxides employing the plasma oscillation theory of solids up to date. Therefore, in this work, we propose a semi-empirical model based on plasma oscillation theory of solids for investigation of anisotropic elastic properties of cubic structured Ln_2O_3 lanthanide series.

2. THEORETICAL INFORMATION AND COMPUTATIONAL TECHNIQUES FOR STATIC ELASTIC CONSTANTS

Static elastic constants (C_{ij}) are very important parameters which define anisotropic elastic properties of the material that undergoes stress, deform and recovers after returning to its original shape and size. For various type of crystal structure of solids, the no. of independent static elastic constants is different. In case of C-type structured sesquioxide crystals, there are three independent static-elastic constant (C_{ij}: C_{11}, C_{12} & C_{44}). Based on semi-empirical linear relations, a number of theoretical linear expressions for static-elastic constant [41] for binary solids and mechanical properties [42] of ternary chalcopyrite structured semiconductors in term of the melting temperature (T_m), Boltzmann's constant (K_B), atomic volume (Ω) and product of ionic charge. Almost in many linear empirical relations [33,40] we have observed that bulk modulus (B) for various type of crystals is related to the product of ionic charge and bond length of a compound as follows -

$$B = A(Z_1 Z_2)d^{-3} \tag{1}$$

Recently, Verma [41] has developed a linear regression relation for elastic stiffness constant C_{ij} for ZB- structured binary solids in term of product of ionic charge and bond length of a compound as -

$$C_{ij} = \delta_{ij} + \gamma_{ij}(Z_1 Z_2)^{\mu_{ij}} d^{-3} \tag{2}$$

Here γ_{ij}, μ_{ij} and δ_{ij} are numerical constant for binary solids. Further, Frost and Ashby [42] have developed an empirical model for the elastic moduli of binary solids in terms of ($K_B T_m/\Omega$) as given as-

$$E = 100 K_B T_m / \Omega \tag{3}$$

$$G = 44 K_B T_m / \Omega \tag{4}$$

Similarly, Verma [43] has developed an empirical relation for elastic stiffness constant (C_{ij}) of tetragonal structured chalcopyrite crystals using ionic charge theory of solids and defined as-

$$C_{ij} = A_{ij}(K_B T_m / (Z_1 Z_2 Z_3)\Omega)^{0.15} \tag{5}$$

Here A_{ij} is the proportionality constant for C_{ij} of $A^{I}B^{III}C^{V}_2$ and $A^{II}B^{IV}C^{V}_2$ chalcopyrite semiconductors. Recently, Kumar et al [44] have proposed polynomial relations for the estimations of electronic, elastic and optical properties of divalent and trivalent rare earth mono-chalcogenide materials in term of their Plasmon energy as a key parameter. According to them-

$$B = K_1 + K_2(\hbar\omega_p) + K_3(\hbar\omega_p)^2 \tag{6}$$

$$E_c = K_4 \exp[K_5(\hbar\omega_p)] \tag{7}$$

In these relations K_1, K_2, K_3, K_4, and K_5 are numerical constants. According to above theoretical information's, it is very clear that static elastic constants (C_{ij}) are also depends upon the plasma energy of the materials. To get better agreement between the available experimental and theoretical data for C-type lanthanide sesquioxide crystals, based on above discussion, we may extend the relations (2) and (5) employing the plasma oscillation theory [32, 35-38] with minor modifications and can be written in the following form as-

$$C_{ij} = D_{ij}(\hbar\omega_p)^s \tag{8}$$

In this relation (9), the numerical value of the proportionality constant depends on the crystal structure. For cubic structured lanthanide series, the value of D_{ij} equal to 0.717, 0.320 and 0.298 for C_{11}, C_{12} and C_{44} respectively and exponent S = 2.0 for all C_{ij} of the materials. Using empirical relation (8), elastic constants (C_{11}, C_{12}, C_{44}) and elastic compliance $S_{ij} = C_{ij}^{-1}$ of Ln_2O_3 are calculated and presented in Table-1 with available theoretical literature [16] for a comparative study. An excellent agreement has been found between them.

The present investigations of C_{ij} for cubic sesquioxides satisfy the mechanical stability conditions defined by Born [45] as

$$(C_{11}\text{-}C_{12}) > 0,\ C_{44} > 0,\ C_{11} > 0,\ C_{12} > 0,\ (C_{11}+2C_{12}) > 0 \text{ and } C_{11} > B > C_{12}$$

These results indicate that the lanthanide sesquioxide crystals are mechanically stable against elastic deformations. For cubic structure crystals, the static elastic constants C_{ij} play an important role to determining the elastic constants such as isotropic bulk modulus (B), compressibility (K=1/B), shear modulus (G) using Voigt-Reuss-Hill (VRH) approximations, Young's modulus (E), Poisson's ratio (ν), Zener anisotropy factor (Z), shear wave constant (C_s), Cauchy Pressure (C^*) and Kleinman internal displacement parameter (ξ) of these materials. The expressions of above parameters are defined in terms of C_{ij} as follows-

$$B = (C_{11} + 2C_{12})/3 \tag{9}$$

Voigt shear modulus,

$$G_v = (C_{11} - C_{12} + 3C_{44})/5$$

Reuss shear modulus,

$$G_R = 5C_{44}(C_{11} - C_{12})/[4C_{44} + 3(C_{11} - C_{12})$$

$$G_H = (G_V + G_R)/2 \tag{10}$$

Young's modulus,

$$E = (C_{11} + 2C_{12})(C_{11} - C_{12})/(C_{11} + C_{12}) \tag{11}$$

Poisson's ratio,

$$\nu = C_{12}/(C_{11} + C_{12}) \tag{12}$$

Zener anisotropic factor,

$$Z = 2C_{44}/(C_{11} - C_{12}) \tag{13}$$

Kleinman parameter,

$$\xi = (C_{11} + 8C_{12})/(7C_{11} + 2C_{12}) \tag{14}$$

Shear wave constant,

$$C_s = (C_{11} + C_{12})/2 \tag{15}$$

Cauchy pressure,

$$C^* = C_{12} - C_{44}) \tag{16}$$

Grüneisen Parameter,

$$\gamma = 3(C_{11} + 2C_{12}) / 2(2C_{11} - C_{12}) = 1.5(1+\nu) / (2-3\nu) \quad (17)$$

Based on elastic moduli E and ν, Lame's coefficients (λ & μ) are computed by the following relations as

$$\lambda = E\nu / (1+\nu)(1-2\nu) \text{ and } \mu = E / 2(1+\nu) \quad (18)$$

On the basis of above relations, the investigated values of static elastic constants and mechanical moduli of the cubic structure lanthanide sesquioxides are presented in the respective Tables along with the available experimental data and other such theoretical reports. We found a good agreement between them. The values of Pugh ratio is equal to 0.556 for all sesquioxides and indicate the information about covalent and ionic behavior of the materials on the basis of their brittle and ductile nature in these solids. The upper limits of Pugh ratio is 1.1 for brittle and 0.60 for ductile nature. It is clear that, if (G/B) ≤ 0.60, the materials are ionic (ductile), otherwise covalent (brittle) in nature.

3. RESULTS AND DISCUSSION

The static elastic constants (C_{11}, C_{12}, C_{44}) and mechanical/elastic moduli are reflecting the important anisotropic elastic properties of cubic structured (with space group Ia3, 206) lanthanide sesquioxides. We have employed an empirical relation for the calculation of C_{ij} of these compounds in term of their Plasmon energy, which play an important role as key parameter. In the present work, the calculated values of C_{ij} employed to the relations (9)-(18) straight forwardly and the values of elastic moduli (B, G, E, K, ν, G/B, $S_{ij}=1/C_{ij}$,) and other parameters (Z, C_s, C^*, λ, μ, ξ, γ) of these compounds are also investigated. We note that the calculated values of C_{ij} from our proposed model are cited in Table-1and are very close to theoretical reports [17] and elastic compliances S_{ij} are also presented in such Table. The static elastic constants (C_{ij}: C_{11}, C_{12}, C_{44}) of these sesquioxides exhibit a linear relationship when plotted on log-log scale against their plasma energy. Bulk modulus is the key parameter of solid-state materials. The values of B computed by well-known relation in term of C_{11} and C_{12} and are cited in Tale-2 with the current theoretical and experimental report [17, 46]. An excellent agreement has been found between them. Voigt-Reuss-Hill approximation is average of the two bounds as lower bound of Voigt and upper bound by Reuss, which yields good estimations for shear modulus (G) and are provided in Table-2 with current theoretical literature. One of them, Young's modulus (E) is a mechanical parameter, which is used to measure the stiffness or hardness of the materials. If the value of E is very high, then the material is stiffer and for low values of E, the material is least stiff to them. Thus, it is very clear from Table-2 that in a series of Ln_2O_3, La_2O_3 is least stiff as compared to all of them, while Lu_2O_3 is much stiffer in them. Poisson's ratio is the constant which is used to differentiate the nature of the materials that it is ductile or brittle. The critical value of Poisson's ratio is 0.33 proposed by Frantsevich [52]. If ν<0.33, the material is brittle and for ν>0.33 the material in ductile nature. The calculated values of Poisson ratio for these compounds are equal to 0.2604 and displays in the Table 3, which show that the brittle nature of studied materials. In this Table, the calculated values of Kleinman parameter (ξ), Lame's coefficient (λ & μ) and Zener anisotropy factor (Z) for cubic sesquioxides are presented here. Zener anisotropy factor (Z) is used to measure the degree of anisotropy in the solid-state structure. For Z=1, the material is completely isotropic, and if Z ≠ 1 the materials are elastically anisotropic in nature. In Table-3 the positive values of the Cauchy pressure for all cubic lanthanide series indicates that the materials are ductile in nature rather than brittle [53].

Table 1. Calculated values of elastic stiffness constants of cubic structured lanthanide sesquioxides

Ln_2O_3	$\hbar\omega_p$ (eV)	Elastic Stiffness Constant C_{ij} (GPa)						Elastic Compliance		
		C_{11}		C_{12}		C_{44}		S_{ij} ($\times 10^{-3}$ TPa)		
		Calc.	Ref.*	Calc.	Ref.*	Calc.	Ref.*	S_{11}	S_{12}	S_{44}
La	16.403	192.91		86.09		80.18		7.2	2.2	12.5
Ce	16.612	197.86		88.30		82.23		7.0	2.2	12.2
Pr	16.818	202.80		90.51		84.28		6.8	2.1	11.9
Nd	17.021	207.72		92.71		86.33		6.6	2.1	11.6
Pm	17.222	212.66	206.9	94.91	94.0	88.38	86.0	6.5	2.0	11.3
Sm	17.422	217.63	213.8	97.12	95.8	90.45	88.6	6.3	2.0	11.1
Eu	17.617	222.52	222.6	99.31	98.4	92.48	92.8	6.2	1.9	10.8
Gd	17.812	227.48	228.7	101.53	98.9	94.54	94.6	6.1	1.9	10.6
Tb	18.004	232.41	235.1	103.73	100.3	96.59	97.1	5.9	1.8	10.4
Dy	18.194	237.34	241.2	105.93	101.4	98.64	99.6	5.8	1.8	10.1
Ho	18.382	242.27		108.13		100.69		5.7	1.8	9.9
Er	18.568	247.20		110.33		102.74		5.6	1.7	9.7
Tm	18.753	252.15		112.54		104.80		5.5	1.7	9.5
Yb	18.935	257.07		114.73		106.84		5.4	1.7	9.4
Lu	19.116	262.00		116.93		108.90		5.3	1.6	9.2

*Ref.[16]

Table-2. Values of the elastic moduli of cubic structured lanthanide sesquoxides with available theoretical and experimental data

Ln_2O_3	Elastic Moduli (in GPa)												
	Bulk Modulus (B)			Shear Modulus(G)						Young's Modulus (E)		Pugh's ratio	Gruneisen Const.
	Calc..	Reported[#]	Expt[#]	G_{VCalc}	Ref[*]	$G_{RCalc.}$	Ref[*]	G_{HCalc}	Ref[*]	Calc	Reported[*]	(G/B)	γ
La	121.69	124.4, 125.6, 133.9		69.47		66.78		68.13		175.10		0.559	1.550
Ce	124.82	135.5, 135.8, 148.5		71.25		68.49		69.87		179.59		0.559	1.550
Pr	127.94	137.0, 148.2, 157.9		73.02		70.20		71.61		184.07		0.559	1.550
Nd	131.04	122.0, 136.9, 150.5		74.80		71.91		73.35		188.54		0.559	1.550
Pm	134.16	131.6[*],129.0,136.0,153.8		76.57	74.2	73.62	71.1	75.09	72.6	193.02	187.4	0.559	1.550
Sm	137.29	135.1[*],136.5,138.3,153.4	116,142,149	78.37	76.8	75.34	73.8	76.85	75.3	197.53	193.6	0.559	1.550
Eu	140.38	139.8[*],143.1, 137.0,156.1	115	80.13	80.5	77.03	77.5	78.58	79.0	201.97	202.7	0.559	1.550
Gd	143.51	142.2[*],144.7,139.7,158.3	134,125,188	81.91	82.7	78.75	80.0	80.33	81.3	206.47	207.9	0.559	1.550
Tb	146.62	145.2[*],139.0,143.7,158.6		83.69	85.2	80.45	82.5	82.07	83.9	210.94	213.8	0.559	1.550
Dy	149.73	148.0[*],148.9,145.3,159.9	150, 191	85.46	87.7	82.16	85.1	83.81	86.4	215.42	219.8	0.559	1.550
Ho	152.84	152.0,145.7,161.6	134,178,206	87.24		83.87		85.55		219.90		0.559	1.550
Er	155.95	157.2,146.1,161.2	155,140,200	89.02		85.58		87.29		224.37		0.559	1.550
Tm	159.07	157.7,161.6,146.6		90.80		87.29		89.04		228.86		0.559	1.550
Yb	162.17			92.57		88.99		90.78		233.33		0.559	1.550
Lu	165.28			94.35		90.70		92.53		237.81		0.559	1.550

*Ref.[17], [#]Ref.[18]

Table 3. In this Table, we present the values of Shear constant (C_s), Cauchy Pressure (C'), Lame's coefficients (λ and μ), Kleinman Parameter (ξ), Zener Anisotropy (Z) and Poisson ratio (ν) of C-type lanthanide sesquioxides and compared with Ab-initio study

Ln_2O_3	Shear Constant		Cauchy Pressure		Lame's Coefficients				Kleinman Parameter		Zener Anisotropy		Poisson Ratio	
	C_S		C^*		λ		μ		ξ		Z		ν	
	Calc	Ref.[*]	Calc	Ref.[*]	Calc	Ref.[*]	Calc	Ref.[*]	Calc	Ref.[*]	Calc	Ref.[*]	Calc	Ref.[*]
La	53.408	------	5.919	------	75.390	------	69.471	------	0.749	------	1.501	------	0.2602	------
Ce	54.778	------	6.071	------	77.324	------	71.252	------	0.749	------	1.501	------	0.2602	------
Pr	56.145	------	6.224	------	79.253	------	73.031	------	0.748	------	1.501	------	0.2602	------
Nd	57.508	------	6.375	------	81.178	------	74.804	------	0.748	------	1.501	------	0.2602	------
Pm	58.875	56.5	6.527	8.0	83.108	82.2	76.581	74.2	0.749	0.76	1.501	1.52	0.2602	0.26
Sm	60.250	59.0	6.677	7.2	85.045	84.0	78.370	76.8	0.749	0.75	1.501	1.50	0.2602	0.26
Eu	61.606	62.1	6.827	5.6	86.963	86.1	80.135	80.5	0.749	0.74	1.501	1.49	0.2602	0.26
Gd	62.978	64.9	6.979	4.3	88.898	87.0	81.918	82.7	0.749	0.73	1.501	1.46	0.2602	0.26
Tb	64.343	67.4	7.131	3.2	90.825	88.4	83.694	85.2	0.749	0.72	1.501	1.44	0.2602	0.26
Dy	65.706	69.9	7.282	1.8	92.752	89.7	85.470	87.7	0.749	0.71	1.501	1.42	0.2602	0.26
Ho	67.073	------	7.434	------	94.679	------	87.245	------	0.748	------	1.501		0.2602	------
Er	68.437	------	7.585	------	96.605	------	89.020	------	0.749	------	1.501		0.2602	------
Tm	69.807	------	7.736	------	98.539	------	90.802	------	0.749	------	1.501		0.2602	------
Yb	71.179	------	7.889	------	100.460	------	92.572	------	0.748	------	1.501		0.2602	------
Lu	72.538	------	8.039	------	102.330	------	94.352	------	0.749	------	1.501	------	0.2602	------

[*]Ref.[16]

Hence, the calculate results indicate that proposed empirical model is quite simple and give us soundness in results for these cubic structure lanthanide sesquioxides and predicts the anisotropic elastic properties of Ln_2O_3 compounds successfully. We have plotted a graph between static elastic constant (C_{ij}; in GPa) and Plasmon energy of the materials shown in Fig.-1. It is clear that C_{ij} trends in these compounds increases on increasing their plasma energy.

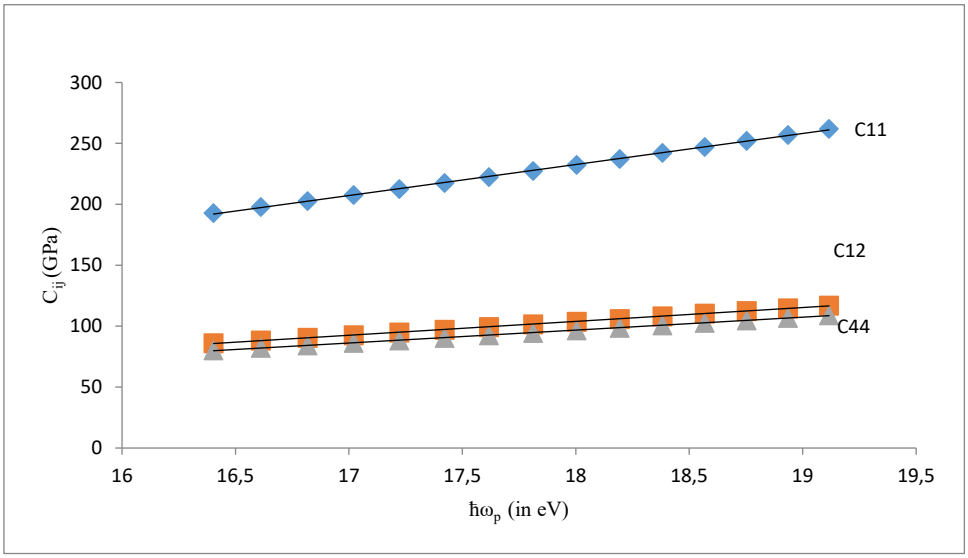

Figure 1. Plot of C_{ij} versus plasmon energy for Ln_2O_3.

4. CONCLUSIONS

On the basis of solid-state theory of plasma oscillations, the anisotropic elastic properties of lanthanide sesquioxides are investigated using the proposed empirical model. From above results and discussions, we have concluded that Plasmon energy of cubic structure sesquioxides is very important parameter which leads to determining three independent elastic stiffness constants (C_{ij}: C_{11}, C_{12}, C_{44}). Elastic moduli of these materials increase on increasing the plasma energy as from $La_2O_3 \rightarrow Lu_2O_3$. In our studied materials, La_2O_3 is least stiff and Lu_2O_3 is stiffer in Ln_2O_3 series. The elastic properties of these compounds allowed us to conclude that the considered materials are elastically anisotropic. In addition, the values of the elastic constants of these materials shows that the cubic structured lanthanide sesquioxides are mechanically stable. Here, the predictions were found to be in good agreement with the available experimental data and theoretical findings. But, unfortunately for many compounds, some predicted values could not be compared due to lacking of availability of experimental results to make a comparison. Finally, it may be seen that the proposed empirical model can easily be extended to cubic sesquioxide crystals for which the work is in progress and will be appearing in forthcoming paper.

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REFERENCES

[1] K.A. Gschneidner, and L. Erying, *Handbook on the Physics and Chemistry of Rare Earths*, Vol. **1-40**, 202 (1978-2010).
[2] S. Jiang, J. Liu, X.-D. Li, Y.-C. Li, S.-M. He, and J.-C. Zhang, Chin. Phys. Lett. **36**(4), 046103 (2019). https://doi.org/10.1088/0256-307X/36/4/046103
[3] J. Łazewski, M. Sternik, P.T. Jochym, J. Kalt, S. Stankov, A.I. Chumakov, J. Göttlicher, *et al*., Inorg. Chem. **60**(13), 9571 (2021). https://doi.org/10.1021 /acs.inorgchem.1c00708
[4] J. Ibanez, J.A. Sans, V. Cuenca-Gotor, R. Oliva, O. Gomis, P. Rodriguez-Hernandez, A. Munoz, *et al*., Inorg. Chem. **59**(14), 9648 (2020). https://dx.doi.org/10.1021/acs.inorgchem.0c00834
[5] S. Jiang, J. Zhang, L. Wang, C. Lin, S. Yan, J. Liu, A. Li, and R. Tai, AIP Advances, **13**, 095018 (2023). https://doi.org/10.1063/5.0164684
[6] S. Jiang, J. Zhang, and S. Yan, AIP Advances, **13**, 055308 (2023). https://doi.org/10.1063/5.0140946
[7] Y. He, M. Chen, Y. Jiang, L. Tang, J. Yu, Y. Chen, M. Fu, *et al*., J. Alloys Compd. **903**, 163806 (2022). https://doi.org/10.1016/j.jallcom.2022.163806
[8] L. Erying, *Handbook on the Physics and Chemistry of Rare Earths*, **3**, 337-339 (1997).
[9] V.P. Zhuze, and A.I. Shelykh, Sov. Phys. Semicond. **23**, 245 (1989).
[10] H.R. Hoekstra, and K.A. Gingerich, Science, **146**, 1163 (1964). https://doi.org/10.1126/science. 146.3648.1163
[11] G. Adachi, and N. Imanaka, Chemical Reviews, **98**, 1479 (1998). https://doi.org/10.1021/cr940055h
[12] M. Rahm, and N.V. Skorodumova, Phys. Rev. **B80**, 104105 (2009). https://doi.org/10.1103 /PhysRevB.80.104105
[13] L. Petit, A. Svane, Z. Szotek, and W.M. Temmerman, Phys. Rev. B, **72**, 205118 (2005). https://doi.org/10.1103/PhysRevB.72.205118
[14] N. Hirosaki, S. Ogata, and C. Kocer, J. Alloys Compds. **351**, 31 (2003). https://doi.org /10.1016 /S0925-8388(02)01043-5
[15] A. Prokofiev, A.I. Shelykh, and B.T. Melekh, J. Alloys Compds. **242**, 41 (1996). https://doi.org/10. 1016/0925-8388(96)02293-1
[16] N. Singh, S.M. Saini, T. Nautiyal, and S. Auluck, J. Appl. Phys. **100**, 083525 (2006). https://doi.org /10.1063/1.2353267
[17] A.K. Pathak, and T. Vazhappilly, Phys. Stat. Sol. (b) **255**, 1700668 (2018). https://doi.org/10.1002 /pssb.201700668

[18] D. Rechard, E.L. Munoz, M. Renteria, L.A. Errico, A. Svane, and N.E. Christensen, Phys. Rev. B, **88**, 165206 (2013). https://doi.org/10.1103/PhysRevB.88.165206
[19] J. Sheng, B.L. Gang, L. Jing, X.W. Sheng, L.X. Dong, L.Y. Chun, T.L. Yun, *et al*., Chin. Phys. Lett. **26**, 076101 (2009). https://doi.org/10.1088/0256-307X/26/7/076101
[20] K.A. Irshad, P. Anees, R. Rajitha, T.R. Ravindran, V. Srihari, S. Kalavathi, and N.V. Chandra Shekar, Journal of Alloys and Compounds **822**, 153657 (2020). https://doi.org/10.1016/j.jallcom.2020.153657
[21] A.F. Andreeva, and I.Y. Gilman, Zh. Prikl. Spectrosk, **28**, 895 (1978). Ref. no. – AIX-10-431358, EDB-79-100351
[22] M.V. Avrashev, N.D. Todorov, and J. Geshev, J. Appl. Phys. **116,** 103508 (2014). https://doi.org/10.1063/1.4894775
[23] S. Jiang, J. Liu, C. Lin, L. Bai, Y. Zhangb, X. Li, Y. Li, *et al*., Solid State Communications **169**, 37 (2013). https://doi.org/10.1016/j.ssc.2013.06.027
[24] V.I. Marchenko, Electronic Structure and Physico Chemical Properties of Refractory Compounds and alloys, **193**, (1980).
[25] M. Shafiq, S. Arif, I. Ahmad, S.J. Asadabadi, M. Maqbool, and H.A.R. Aliabad, J. Alloys Compds. **618**, 292 (2015). https://doi.org/10.1016/j.jallcom.2014.08.171
[26] H. Jiang, P. Rinke, and M. Scheffler, Phys. Rev. B, **86**, 125115 (2012). https://doi.org/10.1103/ PhysRevB.86. 125115
[27] A.S. Verma, Solid State Communication, **149**, 1236 (2009). https://doi.org/10.1016/j.ssc.2009.04.011
[28] D.S. Yadav, and S. P. Singh, Phys. Scr. **82**, 065705 (2010). https://doi.org/10.1088/0031-8949/82/06/065705
[29] D.S. Yadav and A.S. Verma, Int. J. Mod. Phys. B, **26**, 1250020 (2012). https://doi.org/10.1142/ S02179792 12500208
[30] A. S. Verma, S. Sharma, and V.K. Jindal, Mod. Phys. Lett. B, **24**, 2511 (2010). https://doi.org /10.1142/ S0217984910024821
[31] R. Bhati, D.S. Yadav, R.C. Gupta, A.S. Verma, Materials Physics and Mechanics, **51**(5), 90 (2023). http://dx.doi.org/10.18149/MPM.5152023-9
[32] V. K. Srivastava, Phys. Rev. B, **29**(12), 6993 (1984). https://doi.org/10.1103/PhysRevB.29.6993
[33] A.S. Verma, Phys. Scr. **79**, 045703 (2009). https://doi.org/10.1088/0031-8949/79/04/045703; A.S. Verma, N. Pal, B.K. Sarkar, R. Bhandari, and V.K. Jindal, Phys. Scr. **85**, 015705 (2012). https://doi.org/10.1088/0031-8949/85/01/015705
[34] S.K. Gorai, and P. Mahto, Indian J. Phys., **86(4)**, 273 (2012). https://doi.org/10.1007/s12648-012-0053-y
[35] D. S. Yadav and D.V. Singh, Phys. Scr., **85**, 015701 (2012). https://doi.org/10.1088/0031-8949/85/01/015701
[36] D.S. Yadav, J. Alloy. Compds. **507**, 250 (2012). https://doi.org/10.1016/j.jallcom.2012.05.016
[37] D.S. Yadav, J. Mater. Chem. Phys, **3**, 6 (2015). https://doi.org/10.12691/jmpc-3-1-2
[38] R. Bhatti, D.S. Yadav, P. Vershney, R.C. Gupta, A.S. Verma, East European Journal of Physics **1,** 222 (2023). https://doi.org/10.26565/2312-4334-2023-1-29
[39] D.S. Yadav, and A.S. Verma, Int. J. Mod. Phys. B, **26**, 1250020 (2012). https://doi.org/10.1142 /S0217979212500208
[40] N. Yadav, D.S. Yadav, P. Varshney, R.C. Gupta, American Journal of Physics and Applications **11(4),** 80 (2023). https://doi.org/10.11648/j.ajpa.20231104.11
[41] A.S. Verma, Materials Science in Semiconductor Processing, **29**, 2 (2015). https://doi.org/10.1016 /j.mssp .2014.05.033
[42] H.J. Frost, and M.F. Ashby, *Deformation-Mechanism Maps*, (Pergamon, Oxford, (1982).
[43] A.S. Verma, S. Sharma, R. Bhandari, K. Sarkar, and V.K. Jindal, Mater. Chem. Phys., **132**, 416 (2012). https://doi.org/10.1016/j.matchemphys.2011.11.047
[44] V. Kumar, S. Chandra, and J.K. Singh, Indian J. Phys. **3**, 0983 (2017). https://doi.org/10.1007/s12648-017-0983-5
[45] M. Born, and K. Hung, *Dynamics Theory of Crystal Lattices*, (Oxford University Press, Oxford, (954).
[46] D. Richard, L.A. Errico, and M. Rentira, J. Alloys Compds. **664**, 580 (2016). https://doi.org/10.1016 /j.jallcom.2015.12.236
[47] W. Voiget, and Teubner, Lehrbuch Der Kristallphysik Leipzig, Germany, 962 (1928).
[48] A. Reyss, and Z. Angew, Math Mech. **8**, 55 (1929).
[49] R. Hill, Proc. Phys. Soc. A, **65**, 349 (1952). https://doi.org/10.1088/0370-1298/65/5/307
[50] D.G. Pettifor, Mater. Sci. Technol. **8**, 345 (1992). https://doi.org/10.1179/mst.1992.8.4.345
[51] L. Kleinman, Phys. Rev. B, **128**, 2614 (1962). https://doi.org/10.1103/PhysRev.128.2614
[52] I.N. Frantsevich, F.F. Voronov, and S.A. Bokuta, *Handbook in Elastic Constants and Elastic Moduli of Metals and Insulators*, (Naukova Dumka, Kiev, 1982). (in Russian)
[53] Y.F. Li, B. Xiao, Y.M. Sun, L. Gao, S.Q. Ma, and D.W. Yi, J. Phys. Chem. Solids, **103**, 49 (2017). https://doi.org/10.1016/j.jpcs.2016.12.001

ПРУЖНІ ВЛАСТИВОСТІ СЕСКВІОКСИДІВ ЛАНТАНІДУ С-ТИПУ

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У цьому дослідженні ми представили твердотільну теорію плазмових коливань для дослідження анізотропних пружних властивостей, таких як три незалежні статичні константи пружної жорсткості (Cij: C11, C12 і C44) твердих тіл лантаноїдів Ln_2O_3 типу С. Розраховані значення статичних констант пружної жорсткості Ln_2O_3 чудово узгоджуються з теоретичними результатами, отриманими за допомогою методів ab-initio. Значення констант пружної жорсткості (Cij) виявляють лінійну залежність, якщо їх нанести на графік відносно їхніх плазмових енергій і лежать на прямій лінії. Для подальшого вивчення достовірності наявних оцінок модулів пружності та інших параметрів цих матеріалів. Механічні модулі, такі як об'ємний модуль (B), модуль зсуву (G), модуль Юнга (E), коефіцієнт Пуассона (ν), постійна хвилі зсуву (Cs), тиск Коші (C*), коефіцієнт Ламе (λ і μ) , параметр Клейнмана (ξ), параметр Грюнезієна (γ), анізотропна константа Зенера (Z) і співвідношення П'ю (G/B) твердих речовин лантаноїдів також були досліджені. Для полусквіоксидних матеріалів лантаноїдів вперше наведено значення статичних констант пружної жорсткості Cij та модулів пружності. На жаль, у поточному дослідженні для багатьох параметрів цих матеріалів не було знайдено експериментальних результатів для порівняння з нашими теоретичними прогнозами. Отримані оцінки добре узгоджуються з наявними експериментальними даними та іншими теоретичними повідомленнями.

Ключові слова: *пружні властивості; плазмонна енергія; Ln_2O_3*