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ELASTIC, MECHANICAL, THERMAL AND ULTRASONIC STUDIES OF LANTHANUM SELENIDE AT ELEVATED TEMPERATURE

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"together we can and we will make a difference"

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ABSTRACT

The elastic, thermal and ultrasonic properties of Lanthanum Selenide (LaSe) have been computed in the temperature range 300-1000 K at an interval of 50 K. The Second order elastic constants (SOECs) are computed using Coulomb and Born-Mayer potentials. SOECs are being used to evaluate various mechanical and thermal parameters, which provide the valuable information about the future performance of the crystal. Mechanical properties such as Young's Modulus, Bulk modulus, Shear modulus, Zener anisotropy factor, Poisson's ratio and Toughness to Fracture ratio have also been computed. Ultrasonic wave propagation velocity and attenuation of LaSe have also been computed along <100>, <110> and <111> directions. The results discussed and correlated with mechanical and thermo-physical properties. The data of Lanthanum Selenide crystal obtained through different techniques give important and valuable information about internal structure and inherent properties of the crystal.

Keywords: *Nearest neighbor distance, Hardness parameter, Ductile, Brittle, Anisotropic.*

INTRODUCTION

The analysis of behavior of rare-earth compounds under high pressure and temperature provide valuable information about their behavior. The extensive research on rare-earth compounds stems from their remarkable optical, magnetic, thermal, and anomalous phase transition properties, particularly in the context of high-pressure structural phase transitions. [1, 2]. Ultrasonic is a widely used for the investigation of properties of materials under different physical conditions and used to characterize the materials during processing and after production. The anomalous physical properties exhibited by rare earth materials arise from their partially filled *f*-orbitals. Specifically, the highly delocalized *f*-electrons of lanthanum ions interact strongly with the lattice, contributing significantly to these properties. The LaSe have NaCl type structure. The knowledge of ultrasonic attenuation helps in providing insight into the microstructure and associated physical properties such as thermal conductivity, specific heat at higher temperature, higher order elastic constants, existence of phase transition, which helps to predict about the future performance of the materials [3-5]. The ultrasonic velocity obtained through elastic constants serves as a pivotal parameter in ultrasonic characterization, offering insights into crystallographic texture and aiding in determining the Debye temperature. Furthermore, the computed elastic constants enable the derivation of mechanical properties such as Young's modulus, Bulk modulus, Poisson ratio, Anisotropic ratio, Tetragonal moduli, and the Zener anisotropy factor. [6-9].

Theory

In the evaluation of ultrasonic attenuation, second and third order elastic constants (SOECs and TOECs) play an important role. We have calculated SOECs and TOECs using Brügger's definition of elastic constants at absolute zero. The SOECs and TOECs at different higher temperatures are obtained by the method developed by Leibfried and Haln, Slagle, Hiki and Ghate for NaCl-type crystals as the monochalcogenides have well-developed NaCl-type crystal structure. The Lanthanum Monochalcogenides have ionic-metallic type bonding. The total interaction potential is the sum of the long-range Coulomb attractive potential and the short-range Born-Mayer repulsive potential [10-13] and is given as:

$$\varphi_{\mu\nu}(r) = \pm(e^2/r) + A\, exp\,(-r/b)$$

The electronic charge is e, the nearest neighbor distance is *r*, and the ± signs apply to like and unlike

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charges and A and b are the parameters [14-17].

Higher Order Elastic Constants

The elastic energy density for a crystal of a cubic symmetry can be expanded using Taylor's series expension up to quartic terms as:

$U_0 = U_{2+}U_3+U_4$

$= [1/2!]\ C_{ijkl}\ \alpha_{ij}\ \alpha_{kl} + [1/3!] C_{ijklmn}\ \alpha_{ij}\ \alpha_{kl}\ \alpha_{mn} + [1/4!] C_{ijklmnpq}\ \alpha_{ij}\ \alpha_{kl}\ \alpha_{mn}\ \alpha_{pq}$ …. (1)

where $C_{ijkl},\ C_{ijklmn}$ and $C_{ijklmnpq}$ are the SOECs, TOECs and FOECs in tonsorial form; α_{ij} are the Lagrangian strain components; The SOECs, TOECs and FOECs are as given bellow:

$C_{ijkl} = C_{IJ} = (\partial^2 U/\partial\alpha_{ij}\partial\alpha_{kl})_{\alpha=0}$,

$C_{ijklmn} = C_{IJK} = (\partial^3 U/\partial\alpha_{ij}\partial\alpha_{kl}\partial\alpha_{mn})_{\alpha=0}$

and $C_{ijklmnpq} = C_{IJKL} = (\partial^4 U/\partial\alpha_{ij}\partial\alpha_{kl}\partial\alpha_{mn}\partial\alpha_{pq})_{\alpha=0}$

C_{IJ}, C_{IJK} and C_{IJKL} are the SOECs, TOECs and FOECs in Brügger's definition and voigt notations [18].

$C_{IJ} = C_{IJ}^0 + C_{IJK}^{vib}$, $C_{IJK} = C_{IJK}^0 + C_{IJK}^{vib}$, $C_{IJKL} = C_{IJKL}^0 + C_{IJKL}^{vib}$ …. (2)

Mechanical Constants

Using second order elastic constants, mechanical constants like Young's modulus (Y), Bulk modulus (B), Shear modulus (G), Poisson's ratio (V), Zener's anisotropy (A), Tetragonal Shear modulus (Cs). Toughness to Fracture ratio (G/B) also calculated. These parameters are responsible for determining strength, stability and hardness of the material and given as:

$$Y = \frac{9GB}{G+3B} \qquad B = \frac{C_{11}+2C_{12}}{3} \qquad G = \frac{G_V+G_R}{2}$$

$$V = \frac{3B-2G}{6B+2G} \qquad A = \frac{2C_{44}}{C_{11}-C_{12}} \qquad C_s = \frac{C_{11}-C_{12}}{2}$$

….(3)

where $G_v = \frac{C_{11}-C_{12}+3C_{44}}{5}$ $G_R = \frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})}$ ….(4)

Ultrasonic Velocities

along the <100> crystallographic direction

$$V_l = \sqrt{\frac{C_{11}}{\rho}} \qquad V_{s1} = V_{s2} = \sqrt{\frac{C_{44}}{\rho}}$$

….(5)

along the <110> crystallographic direction

$$V_l = \sqrt{\frac{C_{11}+C_{12}+2C_{44}}{2\rho}} \quad V_{s1} = \sqrt{\frac{C_{44}}{\rho}} \quad V_{s2} = \sqrt{\frac{C_{11}-C_{12}}{\rho}}$$

….(6)

along the <111> crystallographic direction

$$V_l = \sqrt{\frac{C_{11}+2C_{12}+4C_{44}}{3\rho}} \qquad V_{s1} = V_{s2} = \sqrt{\frac{C_{11}-C_{12}+C_{44}}{3\rho}}$$

…. (7)

Here l and s corresponds the longitudinal and shear modes of propagation, respectively.

The Debye average velocity V_D is related to V_l, V_{s1} and V_{s2} as:

$\bar{V}_D = \left[\frac{1}{3}\left\{\frac{1}{V_l^3} + \frac{2}{V_s^3}\right\}\right]^{-1/3}$ along <100> and <111> directions and

$\bar{V}_D = \left[\frac{1}{3}\left\{\frac{1}{V_l^3} + \frac{2}{V_{s1}^3} + \frac{1}{V_{s2}^3}\right\}\right]^{-1/3}$ along <110> direction …. (8)

The Debye temperature (θ_D) is given as:

$$\theta_D = \frac{h}{k_B}\left(\frac{3n}{4\pi}\frac{Nd}{M}\right)^{1/3} \bar{V}_D \qquad ….(9)$$

Ultrasonic Attenuation

The Grüneisen parameters $\langle\gamma_j^i\rangle$'s related to SOECs and TOECs and are evaluated using Mason's tables of pure modes and then average is taken. Where j and i are the direction of propagation and mode of propagation respectively.

These parameters directly give Mason's non-linearity coupling constant (D) as:

$$D = 9\frac{\langle(\gamma_j^i)^2\rangle}{Y_2} - \left(\frac{3C_v T}{E_\circ}\right)\frac{\langle\gamma_j^i\rangle^2}{Y_1}$$

…. (10)

where $\langle\gamma_j^i\rangle^2$ are average square Grüneisen number, $\langle(\gamma_j^i)^2\rangle$ are square average Grüneisen numbers, C_v is specific heat per unit volume, T is temperature and $E_\circ$ is the thermal energy density of the crystal.

The thermos-elastic losses and Akhiezer loss (Attenuation due to Phonon-Phonon interaction) are given by:

$$(\alpha/f^2)_{th} = \frac{4\pi^2\ \langle\gamma_j^i\rangle^2\ KT}{2\rho V^5} \quad \text{and} \quad (\alpha/f^2)_{Akh} = \frac{4\pi^2 E_\circ\left(\frac{D}{3}\right)\tau_{th}}{\rho V^3\ (1+\omega^2\ \tau_{th}^2)}$$

…. (11)

In our case $\omega\tau_{th}$ <<1, therefore the relation reduces to,

$$(\alpha/f^2)_{Akh} = \frac{4\pi^2 E_\circ\left(\frac{D}{3}\right)\tau_{th}}{2\rho V^3}$$

…. (12)

The attenuation coefficients for longitudinal and shear waves are given by:

$$(\alpha/f^2)_{Akh.long} = \frac{4\pi^2 E_\circ\left(\frac{D_l}{3}\right)\tau_l}{2\rho V_l^3} \quad \text{and} \quad (\alpha/f^2)_{Akh.shear} = \frac{4\pi^2 E_\circ\left(\frac{D_S}{3}\right)\tau_s}{2\rho V_s^3}$$

…. (13)

where α is the ultrasonic attenuation, f is the frequency, ω is the angular frequency of ultrasonic waves, D_l and D_s are non-linearity coupling constants, τ_l and τ_s are relaxation times, ρ is crystal mass density and V_l and V_s are acoustic wave velocities for longitudinal and shear waves respectively.

The two relaxation times related to thermal relaxation time as

$$\frac{1}{2}\tau_l = \tau_s = \tau_{th} = \frac{3K}{C_v \overline{V_D^2}} \quad .... (14)$$

where τ_{th} is thermal relaxation time, K is the thermal conductivity, C_v is the specific heat per unit volume and $\bar{V}_D$ is the Debye average velocity as given in eq^n (8).

RESULTS

The value of the nearest-neighbor distance (r_0) is 2.9403×10^{-8} cm and the hardness parameter (q) is 0.345×10^{-8} cm for LaSe are given in Table 1. The values of all the elastic constants evaluated from 300-1000 K and are presented in Table 1.

Table 1. The SOECs and TOECs for LaSe in 10^{11} dyne/cm^2

Temp. (K)	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
300	15.890	5.077	5.210	-218.35	-1.033	9.043	8.688	8.739	8.375
400	16.460	5.039	5.216	-216.98	-3.739	9.266	8.792	8.797	8.375
500	17.039	5.001	5.222	-215.63	-6.527	9.488	8.897	8.854	8.375
700	18.205	4.925	5.235	-212.96	-12.212	9.934	9.105	8.968	8.375
1000	19.965	4.811	5.253	-208.99	-20.851	10.602	9.419	9.137	8.375

Table 2. *Y, B, G, Cs* (in 10^{11} dyne/cm^2), *A* and *B/G* (dimension less) for LaSe

Temp. (K)	Y	B	G	V	A	Cs	G/B
300	13.1868	8.6817	5.2881	0.2468	0.9638	5.4062	0.6091
400	13.4546	8.7510	5.4089	0.2437	0.9136	5.7102	0.6180
500	13.7690	9.0140	5.5279	0.2454	0.8677	6.0187	0.6132
700	14.3325	9.3520	5.7580	0.2444	0.7884	6.6397	0.6156
1000	15.1135	9.8755	6.0849	0.2444	0.6933	7.5770	0.6164

Table 3. Ultrasonic wave velocity in 10^5 cm/sec different crystallographic axis for LaSe crystal

Temp (K)	⟨100⟩		⟨110⟩			⟨111⟩	
	V_l	$V_{s1}= V_{s2}$	V_l	V_{s1}	V_{s2}	V_l	$V_{s1}= V_{s2}$
300	4.9984	2.8623	4.9676	2.8623	4.1232	4.9572	2.8979
400	5.0872	2.8640	5.0104	2.8640	4.2375	4.9845	2.9529
500	5.1759	2.8673	5.0536	2.8673	4.3505	5.0122	3.0077
700	5.3501	2.8690	5.1396	2.8690	4.5694	5.0675	3.1150
1000	5.6028	2.8741	5.2667	2.8741	4.8813	5.1498	3.2704

Table 4. Thermal attenuation in 10^{-20} Nps^2 /cm and phonon-phonon attenuation (Akhiezer loss) for longitudinal and shear waves in 10^{-18} Nps^2 /cm for LaSe crystal along different directions

Temp. (K)	$(\alpha/f^2)_{th}$			$(\alpha/f^2)_{Akh}$							
	⟨100⟩	⟨110⟩	⟨111⟩	⟨100⟩		⟨110⟩			⟨111⟩		
	Long.	Long.	Long.	Long.	Shear	Long.	Shear ⟨001⟩	Shear $\langle 1\bar{1}0\rangle$	Long.	Shear $\langle\bar{1}10\rangle$	Shear $\langle 11\bar{2}\rangle$
300	225.40	336.45	318.66	372.77	85.50	373.07	178.56	2144.90	252.94	1340.51	2621.28
400	290.05	454.97	426.03	452.37	109.52	402.91	225.74	2268.49	307.11	1468.29	2841.84
500	320.63	529.29	490.10	465.80	118.63	373.69	241.39	2051.30	316.96	1375.95	2623.45
700	226.11	414.64	376.05	286.34	79.69	93.42	158.14	992.47	197.32	716.73	1311.66
1000	-477.11	-1029.63	-910.68	-511.52	-157.48	-1116.90	-301.71	-1295.27	-366.93	-1049.70	-1784.08

We can see from Table 1 that, the values of C_{11}, C_{44}, C_{112}, C_{123}, C_{144} and C_{166} increases in with temperature, but the values of C_{12} and C_{111} decreases and C_{456} remains constant with temperature. Table 2 shows the variation of various Mechanical constants with temperature. The values Y, B, G, Cs and G/B increases, while the values of V and A decreases with temperature. The variation of ultrasonic velocities and ultrasonic attenuation with temperature shown in Tables 3 and 4. Figs. 1-10 show the variation of ultrasonic wave velocities, attenuation and mechanical parameters with temperature.

Zener's anisotropy is a dimensionless number that is used to quantify the anisotropy for cubic crystals, it quantifies how far a material is from being isotropic, where the value of 1 means an isotropic material. As the Zener anisotropy decreases with temperature, we can say that the anisotropic behavior of LaSe increases with temperature. The tetragonal shear modulus increases with temperature; it suggests that the material becomes stiffer in response to shear stress as temperature increases.

Pugh introduced a straightforward relationship that empirically links the plastic properties of a material to its elastic moduli [19]. Lower values of G/B suggest a propensity for ductility, while higher values indicate brittleness. The demarcation between ductile and brittle materials is determined by a critical value of 0.571. The results obtained show LaSe is brittle in nature.

As the temperature increases from 300K to 1000K, there’s a general trend of increasing velocity for all axes (⟨100⟩, ⟨110⟩, ⟨111⟩) for both longitudinal and shear waves. This is typical behavior for crystalline materials, as higher temperatures allow atoms to vibrate more freely, leading to faster propagation of sound waves. The variation in velocities among different crystallographic axes demonstrates the anisotropic nature of the LaSe crystal.

Thermal attenuation refers to the decrease in the energy or intensity of the waves due to thermal effects within the material. Higher values indicate attenuation that is more significant. Phonon-phonon interactions within the crystal lattice lead to the scattering and absorption of the waves, contributing to attenuation. Attenuation values vary significantly with crystallographic direction, indicating that the attenuation mechanisms differ depending on the orientation of the crystal lattice.The values of ultrasonic attenuation, particularly at higher temperatures (e.g., 1000K), are negative. Negative values of attenuation can occur due to specific characteristics of the material. In this case, they may indicate peculiar behaviors of the crystal at extreme temperatures.

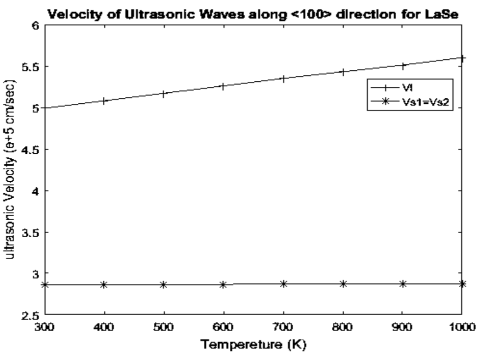

Fig. 1

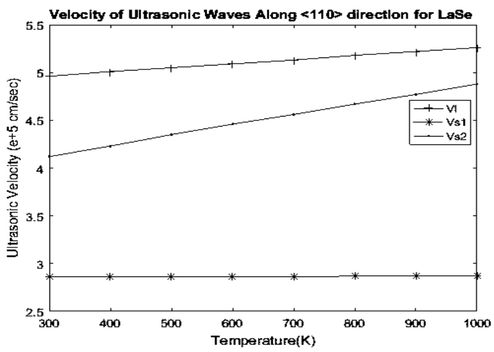

Fig. 2

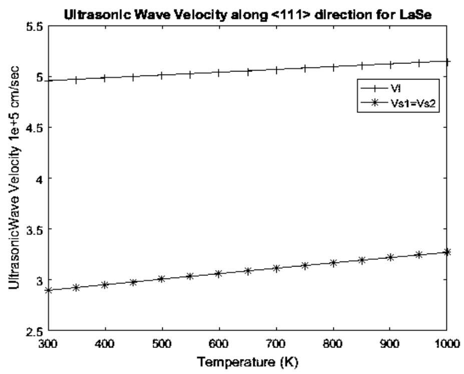

Fig. 3

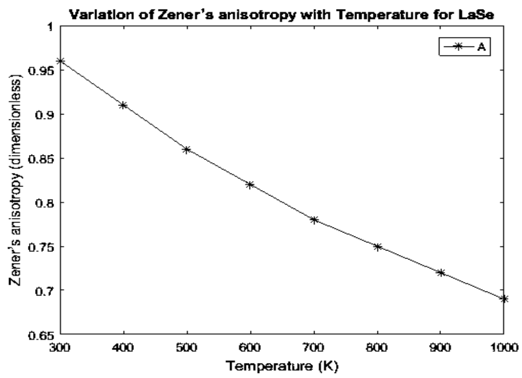

Fig. 4

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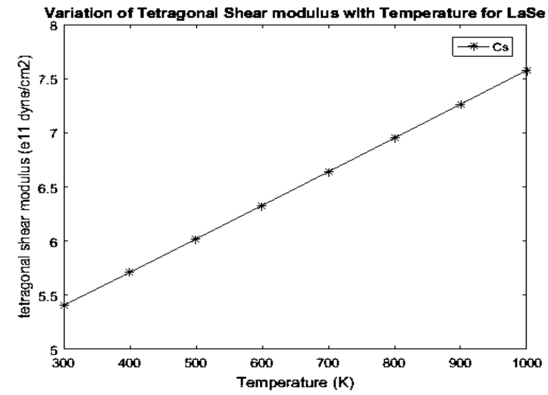

Fig. 5

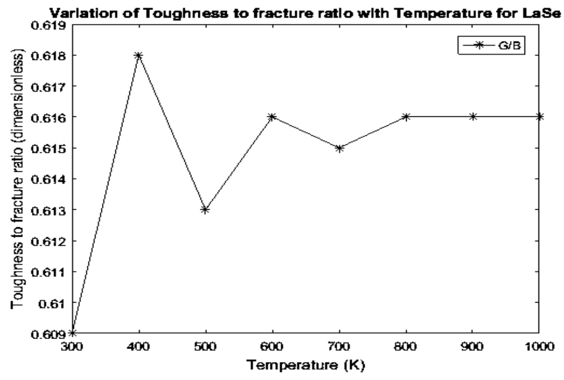

Fig. 6

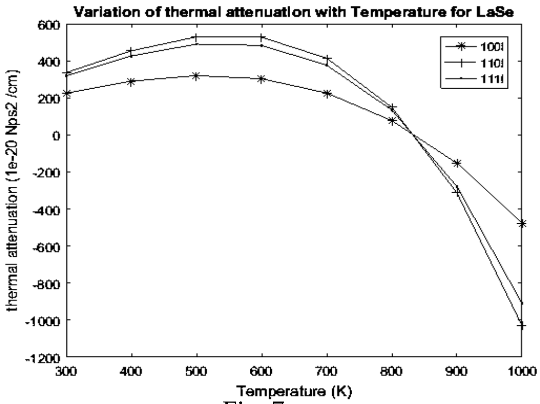

Fig. 7

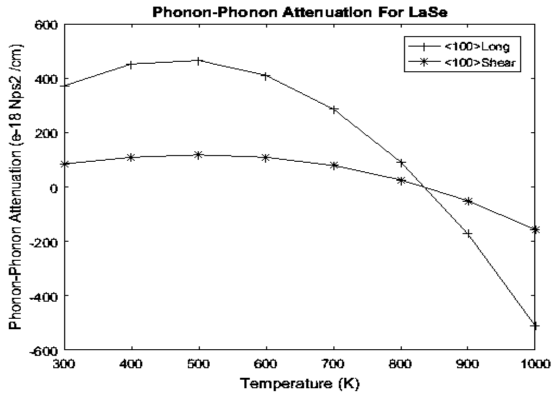

Fig. 8

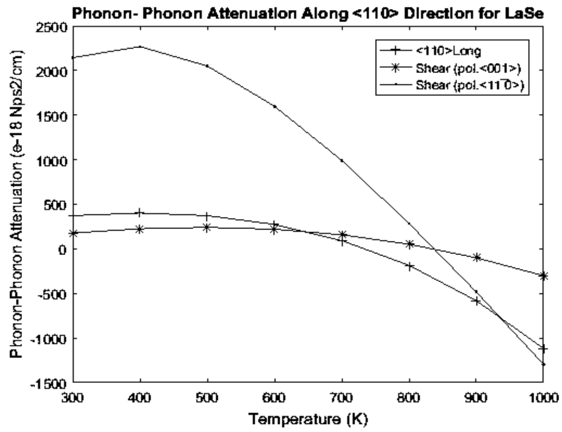

Fig. 9

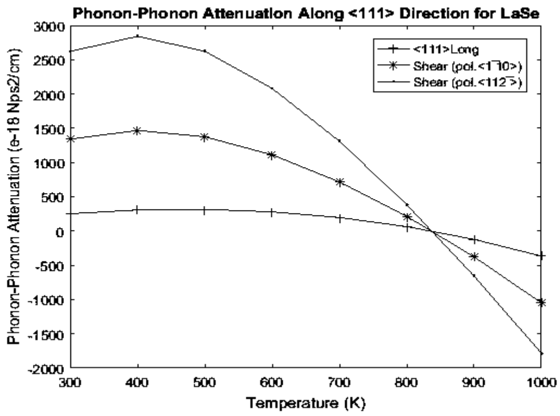

Fig. 10

CONCLUSION

The crystal shows anisotropic nature. The *G/B* ratio for LaSe found to be 0.6091-0.6180, which satisfy its brittle character. The elastic, mechanical, thermal and ultrasonic investigation of LaSe may be useful for further study, reserach and in the industries [20-24]. Anisotropic factor *A* found to be smaller than unity for LaSe it is completely anisotropic material [25]. The temperature range taken is 30-1000 K, the variation of parameters in Fig 1-5 shows the linear variation which indicates the same passion and verifies the theoretical approach. All the values of thermal and phonon-phonon attenuations decreases with temperature. The high temperature data computed in this paper will be beneficial to other researchers engaged in similar studies [26-29]. LaSe's sensitivity to external stimuli, such as temperature and mechanical stress, could be used in sensor and detector technologies. For example, LaSe based sensors could be employed in environmental monitoring, aerospace applications, and industrial process control [30, 31], where precise measurements are critical.

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