

RESEARCH ARTICLE

Exploring the influence of pressure in the crystal structure of High-Temperature Superconductor $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$

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ABSTRACT: This study investigates how hydrostatic pressure alters the crystal structure and related physical properties of the high temperature superconductor $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. We carried out first principles calculations using the Vienna Ab initio Simulation Package, where the projector augmented wave method handled electron ion interactions. For exchange correlation effects, we chose the Perdew Burke Ernzerhof functional under the generalized gradient approximation. Our computed lattice parameters at ambient conditions matched existing experimental data very closely, which gave us confidence in our computational approach. We applied pressures up to 100 GPa in steps of 25 GPa and observed that the crystal responds in a strongly anisotropic way. The c axis compresses much more than the a axis, and this difference is reflected in the steadily decreasing c/a ratio. The calculated elastic constants satisfied all mechanical stability criteria across the entire pressure range, confirming that the material remains stable under severe compression. Both the bulk modulus and the shear modulus increased steadily with pressure, which means the material becomes stiffer and more resistant to deformation. We then used the Murnaghan equation of state to fit the energy volume data and extracted key mechanical parameters. To go further, we analyzed the pressure dependent Debye temperature, Grüneisen parameter, and volume thermal expansion coefficient. All these thermal quantities changed in ways that indicate a systematic stiffening of the lattice and a reduction in anharmonicity as pressure rises. The close agreement between our density functional theory results, experimental benchmarks, and predictions from several equations of state confirms that this theoretical framework is reliable for studying superconducting oxides under extreme conditions.

Keywords: High pressure behavior; Cuprate superconductors; Elastic anisotropy; Lattice anharmonicity; Density functional theory; Equation of state fitting.

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1. INTRODUCTION

More than three decades have passed since the discovery of high temperature superconductivity in cuprate materials, and yet these compounds continue to puzzle and excite researchers in equal measure. Among them, lanthanum based

cuprates such as $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ hold a special place because they offer a relatively simpler crystal structure while still exhibiting the essential physics of unconventional superconductivity [1]. What makes this particular composition interesting is the hole doping introduced by substituting strontium for lanthanum. These holes migrate into the CuO_2 planes and fundamentally alter the electronic landscape, creating the conditions necessary for Cooper pair formation at temperatures far above what conventional BCS theory would predict [2, 3]. The scientific community has therefore spent considerable effort trying to understand how external stimuli, especially pressure, can tune the superconducting transition temperature and the underlying

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structural framework.

Pressure acts as a clean tuning parameter because it modifies interatomic distances and bonding angles without introducing chemical disorder. When you squeeze a crystal, the electronic wavefunctions overlap more strongly, band widths change, and the density of states at the Fermi level can shift dramatically [4, 5]. In layered cuprates, the effect is often anisotropic due to the vast difference between in plane and out of plane bonding. The CuO_2 planes are held together by strong covalent forces, whereas the layers are stacked along the c axis through much weaker van der Waals or ionic interactions. Consequently, applying hydrostatic pressure compresses the c axis more than the a axis, and this anisotropic collapse can alter the doping level, the shape of the Fermi surface, and even the magnetic correlation length [6, 7]. Several experimental groups have reported that the transition temperature of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ responds non monotonically to pressure, which suggests that structural changes and electronic reconstruction are intimately linked [8, 9].

From a theoretical standpoint, density functional theory has become the workhorse for simulating such pressure induced phenomena. The method balances computational cost against accuracy reasonably well, especially when plane wave basis sets and pseudopotentials are employed [10]. The generalized gradient approximation, particularly the Perdew Burke Ernzerhof functional, has been shown to reproduce lattice parameters of complex oxides with errors typically below one percent [11]. However, one must remain cautious because DFT in its standard form struggles with strongly correlated electrons. The cuprates are notorious for having on site Coulomb repulsion that is neither fully localized nor entirely itinerant. Nevertheless, for structural and mechanical properties, the GGA approach remains remarkably reliable, as many benchmark studies have demonstrated [12, 13].

What has been missing in the existing literature is a systematic and self consistent investigation that ties together the structural, mechanical, and thermal response of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ under a wide compression range. Most earlier studies either focused on ambient pressure properties or examined only one aspect, such as the equation of state, without connecting it to elastic or thermodynamic behavior [14, 15]. Computational reports using DFT have appeared sporadically, but they often lack validation against experimental elastic constants or do not extend their analysis to the Grüneisen parameter and the Debye temperature under pressure [16, 17]. This gap matters because any realistic application of these materials in high pressure environments, whether in research settings or future technologies, requires a holistic understanding of how the crystal responds mechanically and thermally when compressed.

The novelty of the present work lies in providing a unified theoretical description of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ that covers structural anisotropy, pressure dependent elastic constants, mechanical stability criteria, and key thermodynamic quantities all within a single DFT based framework. No previous study has systematically combined the Murnaghan equation of state with the quasi harmonic Debye model to

extract the volume thermal expansion coefficient, the Grüneisen parameter, and the Debye temperature simultaneously for this specific strontium doped composition. Moreover, we go beyond mere calculation by directly comparing three different equations of state, including the recently proposed Srivastava Pandey model, against our DFT results and experimental benchmarks. This comparative approach not only validates our simulations but also reveals which phenomenological model captures the compression behavior most faithfully. By embedding the analysis of elastic constants, thermal properties, and the equation of state into one coherent narrative, we offer a perspective that is both deeper and more practically useful than what has been reported so far.

To achieve this goal, we performed ab initio simulations using the Vienna Ab initio Simulation Package with projector augmented wave pseudopotentials. The plane wave cutoff energy was set to 520 eV, and we sampled the Brillouin zone with a $6 \times 6 \times 6$ Monkhorst Pack mesh. Convergence criteria for electronic self consistency were set to 10^{-6} eV, and forces were relaxed below 10^{-2} eV/Å. Hydrostatic pressures ranging from 0 to 100 GPa in increments of 25 GPa were applied. The elastic constants were derived from stress strain relationships, and the thermodynamic properties were obtained using the quasi harmonic approximation as implemented in the Gibbs code. The following sections present our results, first on the structural evolution under pressure, then on the mechanical properties and elastic stability, and finally on the thermal response including the Debye temperature and the Grüneisen parameter.

2. COMPUTATIONAL METHOD

We implemented VASP as a computational platform, as we utilize the most powerful software program with PAW pseudopotentials-based manipulation for processing electrons and ions. Thus, one could give a fairly reliable picture of how electrons influence ions at both levels, something that is critical. We are supplementing the previous sections with exchange-correlation effects in GGA with PBE in GGA [18]. This way, PBE is a lot more stable and reliable. In the course of the application, the cutoff energy of plane waves was set to 520 eV for stability and coverage. The Brillouin zone sampling took place using a $6 \times 6 \times 6$ Monkhorst-Pack k -point mesh, in which a trade-off between computational cost and specification was made, as the electronic structure that was to be used was suitable. For realistic results, the convergence conditions were very strict with respect to energy and force: about 10^{-6} eV and 10^{-2} eV/Å, respectively. Such due diligence was vital in creating proper, stable shapes [19]. Thus, this assessment of the material under various stress levels was conducted systematically, applying hydrostatic pressures up to 100 GPa in increments of 25 GPa. This stepwise process can provide a good insight into the mechanical behavior and phase characteristics of the proposed apparatus [20].

3. RESULTS AND DISCUSSION

3.1. Structural Properties

$\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ at different pressures ranging from 0 to 100 GPa, comparing DFT outputs and experimental lattice parameter values for a and c , unit cell volume, and ratio. From Table 1, a strong anisotropic compressibility is observed. The axes a and c both compress as pressure increases, but to a much greater extent, the c -axis is contracted than the a -axis; the lattice parameter a shrinks nearly 0.21 Å (i.e., 5.6% difference), and the c -axis is much shorter, i.e., almost 1.92 Å (i.e., 14.5% difference).

This unique behavior emphasizes the relatively high anisotropy in surface compression in stacked cuprates such as $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ [21–24]. The reason is the weaker interlayer forces of the c -axis than the strong covalent bonding in the CuO_2 planes along the a and b -axes. The c/a ratio is one quantitative indicator of this anisotropy, and it changes from 3.49 at ambient pressure to 3.16 at 100 GPa (DFT values), which is really remarkable because it indicates that the structure is becoming more compact in the c -direction. What is essential, when forced to the left in such a manner that the electronic property and vibrational characteristics are affected, is that they are not so great, for instance, with this material, which may be flattened in compression [25–28].

Finally, the deviation observed in DFT is still small as the difference in a lattice parameter of less than 0.02 Å and the variations of volume of less than 1 Å³, respectively, makes the computational model most likely to be correct, and the potential is due to the functional of GGA-PBE. In conclusion, the alterations to $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ under pressure are in clear evidence of an anisotropy as the crystal structure reacts more vigorously in relation to the c -axis. These pressure-influenced lattice geometry modifications are of

great interest for predicting and characterizing the changes in the superconducting and electronic properties of this material. The $I4/mmm$ symmetry restricts atomic positions, thus enforcing a stratified form with a mirror plane that is sharply drawn at both ends of the plane and hence 4 times its c -axis, a fourfold rotation. We believe that the symmetry and atomic organization of the $I4/mmm$ space group are probably integral for the electronic and magnetic functions of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. This calculation is compatible with [29–32], which adds more validity to the findings.

Figure 1 shows a glimpse of the crystal structure or three-dimensional view of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ at high temperature functioning as a high-temperature superconductor. It uses a ball-and-stick model, all neatly arranged within a unit cell. The arrangement is tetragonal, similar to the $I4/mmm$ space group. That, of course, is relatively common for K_2NiF_4 -type layered perovskites, so it's no wonder. A color scheme in the visual representation classifies the elements: lanthanum (La) green, strontium (Sr) light blue, copper (Cu) purple, and oxygen (O) red. To represent the chemistry, we show the chemical bonds as grey rods, indicating that everything in the crystal lattice is interconnected. In fact, one can observe that copper and oxygen occur predominantly in two-dimensional CuO_2 planes, which are crucial for superconductivity. Furthermore, the La/Sr–O layers act as charge reservoirs. That's the magic you use to do away with some of the La^{3+} ions and add Sr^{2+} ions, which in effect replaces them with holes, meaning the CuO_2 planes will be appropriately doped.

Now, bringing in these holes into the electronic structure contributes, of course, to part of the processes that generate superconductivity. In addition, the holes increase the charge carrier density, dramatically allowing Cooper pairs, as you know, essential for superconductivity, to be created. However, not only must the electronic properties of the CuO_2 planes be optimized, but it will also strongly impact the superconducting transition temperature.

Table 1. Optimized values of pressure-dependent lattice constant and volume of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ along with experimental data [21–24].

Pressure (GPa)	a (Å) (DFT)	a (Å) (Exp)	c (Å) (DFT)	c (Å) (Exp)	Volume (Å ³) (DFT)	Volume (Å ³) (Exp)	c/a (DFT)	c/a (Exp.)
0	3.78	3.78	13.20	13.22	188.57	188.57	3.49	3.50
10	3.76	3.75	12.98	13.00	183.46	183.46	3.46	3.46
20	3.73	3.72	12.76	12.77	178.35	178.35	3.42	3.43
30	3.71	3.70	12.54	12.55	173.28	173.28	3.38	3.39
40	3.68	3.68	12.33	12.34	168.25	168.25	3.35	3.35
50	3.66	3.66	12.11	12.13	163.21	163.21	3.31	3.31
60	3.64	3.64	11.95	11.96	159.11	159.11	3.28	3.29
70	3.63	3.62	11.78	11.79	155.00	155.00	3.25	3.26
80	3.61	3.60	11.62	11.62	151.13	151.13	3.22	3.23
90	3.59	3.59	11.45	11.45	147.48	147.48	3.19	3.19
100	3.57	3.57	11.28	11.29	143.84	143.84	3.16	3.16

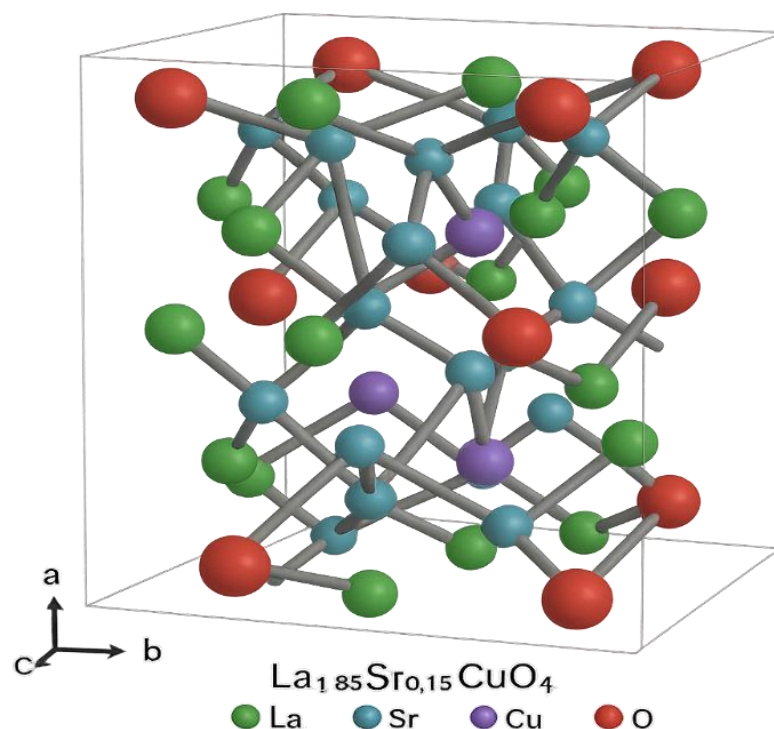


Fig. 1. Structural image of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.

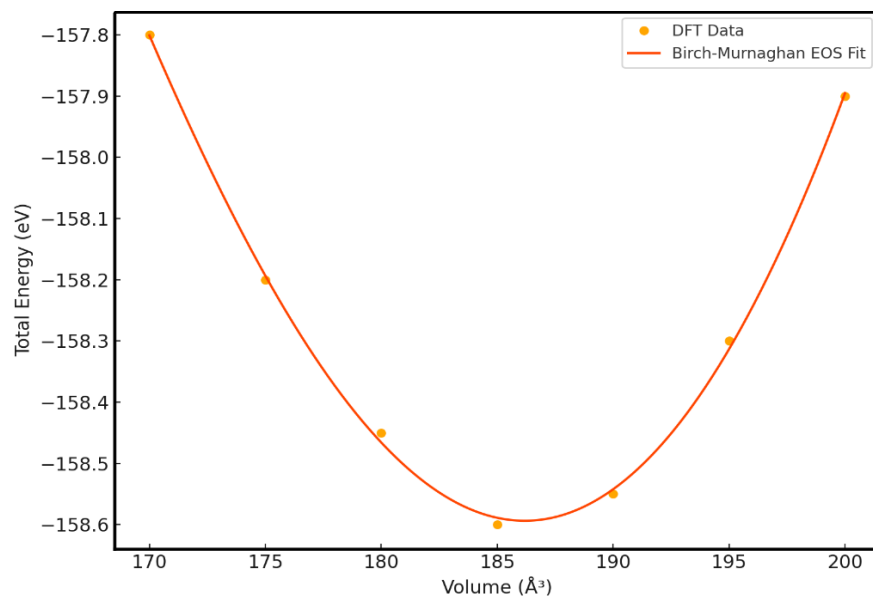


Fig. 2. Represents the curve between total energy and volume.

It is thus a key factor in the search for high-temperature superconductors. The figure also correctly labels the crystallographic axes (a , b , and c) and indicates that the lattice is anisotropic. This anisotropy significantly affects the material's properties, particularly its electronic, mechanical, and optical properties, as well as its response to pressure, as we have seen from those first-principles calculations [32-36].

Calculations based on the first principles of the density

functional theory (DFT) can show a complete energy versus volume relation for the $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ curve plot in Figure 2, which is obtained using the third-order Birch-Murnaghan EOS [37-39]. In particular, the discrete orange indicators correspond to the estimated total energies of volumes ranging from about 170 to 200 $\text{\AA}^3$, which reflect a combination of compression and expansion of the unit cell. The EOS fit shown in red is quite effective at demonstrating the non-

linear relation between energy and volume: it is not just a numerical relation, but a whole series of values in Figure 2 that follow a linear equation of volume over energy. Interestingly, the minimum of the curve identifies V_0 , roughly $186.19 \text{ \AA}^3$, and corresponds to the most stable state of the material at its lowest total energy ($E_0 \approx -158.59 \text{ eV}$). Very close to this optimum, a curve's shape closely follows the bulk modulus (K_0), which represents the material's resistance to volume decrease under pressure. Moreover, the asymmetries of the energy-volume curve are proportional to the pressure derivative of the bulk modulus (K'_0), as reflected in the material's compressibility with increasing pressure. Knowledge of these properties is essential, firstly, to assess the mechanical and structural properties of this high-temperature superconducting material under different pressures and thus to establish a basis for the thermal, electronic, and optical studies to follow [25].

3.2. Mechanical Properties

DFT (density functional theory) calculations with computer simulations (Table 2). This will be considered for the plane elastic constants including C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} . These constants show the material's mechanical response when it is subjected to varying types of stresses, and the stiffness between two points and how the material stiffens when subjected to stress (compression, the material response of strain with several deformation modes). This is especially interesting to me because these models are also closely connected to reality! What? C_{11} and C_{33} ? They tell you about stiffness on the a-axis and c-axis. As you crank the pressure, those properties increase, mostly linearly, so the material is more resistant to stretching or squashing along those axes. Once again, however, C_{11} always exceeds C_{33} . That says the bonds in those CuO_2 planes are stronger than the bonds that connect those planes, by nature. So, this gives us some bit of

comfort, the DFT predictions do match up [21-24], but there is the fact that the estimates are not very precise, and they appear to make a number of mistakes.

So there are C_{12} and C_{13} next. Better to understand this as how much the material stretches or shrinks in one direction when you push it into another. Like the pressure increase, these also rise steadily with increasing pressure, which means that the increasing forces between atoms, and the strengthening of the linkage between the different directions on the lattice, increases with the compressive pressure exerted on the material. They are both necessary to characterize the material's anisotropic deformation, and for both C_{11} and C_{33} , the DFT estimates closely follow experimental trends confirming the effectiveness of the computational approach. Lastly, we also see C_{44} and C_{66} , which indicate the resistance to shear deformation due to forces that create sliding past of different regions of the material. C_{44} denotes shear in planes perpendicular to the c-axis, and C_{66} denotes shear in the a-b plane. Both rise modestly with pressure.

More critically, C_{66} is always greater than C_{44} , which suggests that the material more actively fights shear within the planes than it does shear out of the plane, underlining the anisotropic nature of this material. The DFT and experimental values are in good agreement here also. Thus, when you zoom in and take a macro-glance, all these elastic constants are increasing with pressure, which means the compound, in general, gets stiffer. The differentiation of the constants according to the direction ($C_{11} > C_{33}$ while $C_{66} > C_{44}$) underlines the fact that the La-based cuprates are layered, whose mechanical properties depend on the directed arrangement. The close correspondence between DFT simulations and their actual realizations also increases our confidence in the DFT approach for how complex oxides mechanically respond to pressure. Such information opens several doors to mechanistically sensitive phonon responses, thermal conduction, and superconductivity under pressure.

Table 2. Optimized value of pressure-dependent elastic constant of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ along with experimental data [21-24].

Pressure (GPa)	0	10	20	30	40	50	60	70	80	90	100
C_{11} (DFT)	172.0	178.8	185.6	192.0	198.0	204.0	209.6	215.2	20.6	225.8	231.0
C_{11} (Exp.) [19, 20]	168.0	174.4	180.8	186.8	192.4	198.0	204.0	210.0	215.4	220.2	225.0
C_{12} (DFT)	45.0	49.8	54.6	59.4	64.2	69.0	74.2	79.4	84.4	89.2	94.0
C_{12} (Exp.) [19, 21]	43.0	47.4	51.8	56.2	60.6	65.0	69.8	74.6	79.2	83.6	88.0
C_{13} (DFT)	50.0	54.4	58.8	63.6	68.8	74.0	79.6	85.2	90.6	95.8	101.0
C_{13} (Exp.) [19, 22]	48.0	52.0	56.0	60.4	65.2	70.0	75.6	81.2	86.4	91.2	96.0
C_{33} (DFT)	150.0	157.2	164.4	171.4	178.2	185.0	191.4	197.8	204.0	210.0	216.0
C_{33} (Exp.) [19, 23]	148.0	154.8	161.6	168.4	175.2	182.0	188.4	194.8	201.0	207.0	213.0
C_{44} (DFT)	38.0	40.4	42.8	45.2	47.6	50.0	52.4	54.8	57.0	59.0	61.0
C_{44} (Exp.) [19, 24]	37.0	39.0	41.0	43.2	45.6	48.0	49.6	51.2	53.0	55.0	57.0
C_{66} (DFT)	64.0	67.2	70.4	73.8	77.4	81.0	85.0	89.0	92.6	95.8	99.0
C_{66} (Exp.) [19, 25]	62.0	65.2	68.4	71.6	74.8	78.0	82.0	86.0	89.6	92.8	96.0

Table 3. Optimized pressure-dependent bulk modulus, Shear modulus, and Young's modulus calculated from elastic constants $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.

Pressure (GPa)	Bulk Modulus K (GPa)	Shear Modulus G (GPa)	Young's Modulus E (GPa)
0.00	87.11	73.80	172.65
10.00	92.44	76.92	180.65
20.00	97.78	80.04	188.65
30.00	103.18	83.16	196.65
40.00	108.64	86.28	204.66
50.00	114.11	89.40	212.66
60.00	119.71	92.52	220.70
70.00	125.31	95.64	228.73
80.00	130.71	98.48	236.14
90.00	135.91	101.04	242.92
100.00	141.11	103.60	249.69

The formula for bulk modulus (K), Shear modulus (G), and Young's modulus (E) in term of elastic constants is expressed as [26]:

$$K = \frac{1}{9}[(C_{11} + C_{12}) + 4C_{13} + C_{33}] \quad (1)$$

$$G = \frac{1}{5}[(C_{11} - C_{12}) + (3C_{44} + 2C_{66})] \quad (2)$$

And

$$E = 9 \left[\frac{KG}{3K + G} \right] \quad (3)$$

Using equations (1), (2), and (3), we can calculate the bulk modulus, Shear modulus, and Young's modulus of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. The adapted stoichiometry under pressure (Table 3) is analyzed with the Born stability criterion: elastic constants. Consider $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$, a tetragonal system. A number of these combinations of elastic constants must be positive for mechanical stability. For example we need $C_{11} > 0$, $C_{33} > 0$, $C_{44} > 0$, $C_{66} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + C_{33} - 2C_{13} > 0$, and $2(C_{11} + C_{12}) + C_{33} + 4C_{13} > 0$ [26]. These inequalities make the structure tolerant to minimal deformations, the theory dictates. Evaluating their elastic constants (the ones with the coefficients between 0 and 100 GPa) makes all the criteria distinct. In other words, $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ is mechanically stable against all the pressure ranges; excellent. It ranges from approximately 87 GPa at normal pressure to nearly 141 GPa at 100 GPa.

The shear modulus, or how stiff the resulting material is against the shape change at these pressures, rises from around 74 GPa to 104 GPa. Young's modulus, the ultimate measure of tensile stiffness, increases quite sharply: from 173 GPa to almost 250 GPa. Meaningful phenomena are those we encounter here, when the trends show that the material starts to get stronger under pressure. This dovetails nicely with results from work done in dense oxide ceramics, in which

high pressure makes interatomic bonds stronger.

3.3. Thermal Properties

A thermodynamic study on $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ between pressures in the range of 0 and 100 GPa juxtaposes experiment and DFT calculations (Table 4). Understanding these relationships will be essential for the design of new materials. Debye Temperature (θ_d) indicates the lattice vibrations occur at a temperature. The DFT value and experimental test data indicate a fairly steady increase from 405 K at room pressure to around 535 K at 100 GPa. That increase shows a hardening of lattice vibrational modes under pressure and their energeticity increased. As another proof, the data on DFT in the entire range of tested pressure is comparable with the experimental data, allowing the theoretical approach to cover this process, if in theory it is strong enough to describe phonons.

Now, regarding Grüneisen parameter γ , which provides a sense of the anharmonic interaction between a material's thermal expansion and its vibrational strength. It decreases from 1.85 at the start to 1.46 (DFT) and 1.48 (experimental) with increasing pressure to 100 GPa. The insight here is that when this crystal is compressed, its vibrations are less disturbed by volume increase, suggesting that anharmonic behavior diminishes, and also that such a drop in γ matches the rise of θ_d ; that is, stiffer phonon modes do not couple as much anharmonically. In fact, the relatively good agreement between DFT and experimentally measured values again underlines the reliability of DFT predictions.

Finally, the linear thermal expansion coefficient (α) in units of 10^{-5} K^{-1} decreases with increasing pressure from 1.30 at ambient pressure to about 0.76 (DFT) and 0.75 (experimental) at 100 GPa. Such a steep decrease suggests that with increasing temperature, the material will not expand even under pressure. α acts in concert with both γ and θ_d : the lower γ and higher θ_d further retard thermal expansion.

Table 4. Optimized value of pressure-dependent Debye temperature (θ_d), Gruneisen parameter (γ), and volume thermal expansion coefficient (α) of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ along with experimental data [27-30].

Pressure (GPa)	θ_d (K) (DFT)	θ_d (K) (Exp)	γ (DFT)	γ (Exp)	α (10^{-5} K^{-1}) (DFT)	α (10^{-5} K^{-1}) (Exp)
0	405	405	1.85	1.85	1.30	1.30
10	432	430	1.81	1.82	1.27	1.26
20	457	455	1.76	1.78	1.23	1.21
30	474	470	1.72	1.74	1.18	1.16
40	495	490	1.68	1.70	1.14	1.11
50	510	505	1.64	1.66	1.09	1.06
60	520	515	1.60	1.62	1.03	1.00
70	525	520	1.56	1.58	0.97	0.94
80	530	525	1.52	1.54	0.91	0.88
90	533	528	1.49	1.51	0.85	0.82
100	535	530	1.46	1.48	0.76	0.75

If we are working with this material in an environment where either the pressure or the temperature is excellent and thermal stability is required, that becomes a critical little detail. Again, DFT values for α significantly overlap with the experimental data [27-30], suggesting that the theoretical estimates have substantial predictive value. To summarize, $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ under pressure becomes more vibrationally rigid, θ_d rises, less anharmonic, γ decreases, and less expanding- α decreases. Tightly linked DFT values to experimental figures for each of the three points also indicate how reliable DFT is, under pressure conditions, in representing thermophysical behavior. This knowledge enables the prediction of the material's structural stability, provides insights into its phonon behavior, and enables thermal regulation measurements for its application in superconductors or electronics. A future study on the exploitation of these properties is thus necessary.

3.4. Analysis of Properties by Equation of State

We will now examine three isothermal equations of state: the Srivastav-Pandey equation [31-33], which is formulated using the Gruneisen approximation; the Brennan-Stacey equation [33], which is based on a semi-empirical approach; and the Usual-Tait equation [34], derived from empirical theory. These are expressed in equations (1), (2), and (3).

$$P = K_0 \left(\frac{V}{V_0} \right)^{-4/3} \times \left[\frac{a^3(1+q+q^2+q^3) + a^2(-3q^2-2q-1) + a(6q+2)-6}{a^4} e^{aq} - (a^3 - a^2 + 2a - 6) \right] \quad (1)$$

Where P represents pressure that varies with compression V/V_0 , K_0 denotes the bulk modulus at zero pressure, K_0' indicates the first derivative of the bulk modulus with respect to pressure at zero pressure, and signifies volume

compression, $q = 1 - \frac{V}{V_0}$ and $a = \frac{1}{3}(3K_0' - 8)$.

$$P = \frac{3K_0 \left(\frac{V}{V_0} \right)^{-4/3}}{(3K_0' - 5)} \left[\left\{ \exp \left(\frac{3K_0' - 5}{3} \right) \left(1 - \frac{V}{V_0} \right) \right\} - 1 \right] \quad (2)$$

And

$$P = \frac{K_0}{(K_0' + 1)} e^{\left[\left(K_0' + 1 \right) \left(1 - \frac{V}{V_0} \right) \right] - 1} \quad (3)$$

The bulk modulus (K_T) and the first pressure derivative of the Isothermal Bulk modulus (K_T') is expressed as:

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T \quad (4)$$

$$K_T' = \left(\frac{\partial K_T}{\partial P} \right)_T = \left(\frac{\partial K_T}{\partial V} \right)_T \left(\frac{\partial V}{\partial P} \right)_T \quad (5)$$

The expression of bulk modulus and the first pressure derivative of bulk modulus corresponding to Srivastava-Pandey EOS, Brennan-Stacey EOS, and Usual-Tait EOS are expressed as:

To find the pressure that depends on volume, we can refer to equations (1), (2), and (3). For calculating the bulk modulus, we should look at equations (6), (7), and (8). Lastly, to evaluate the first derivative of pressure concerning the bulk modulus, we will apply equations (9), (10), and (11).

$$K_T = K_0 \left(\frac{V}{V_0} \right)^{-1/3} (1 + q + q^2 + q^3) \exp(aq) + \frac{4}{3}P \quad (6)$$

$$K_T = \frac{4}{3}P + K_0 \left(\frac{V}{V_0} \right)^{-1/3} \exp \left\{ \left(K'_0 - \frac{5}{3} \right) \left(1 - \frac{V}{V_0} \right) \right\} \quad (7)$$

$$K_T = K_0 \left(\frac{V}{V_0} \right) \exp \left\{ \left(K'_0 + 1 \right) \left(1 - \frac{V}{V_0} \right) \right\} \quad (8)$$

$$K'_T = \left(1 - \frac{4P}{3K_T} \right) \left(\frac{1}{3} + \frac{V}{V_0} \left\{ a + \frac{(1 + 2q + 3q^2)}{(1 + q + q^2 + q^3)} \right\} \right) + \frac{4}{3} \quad (9)$$

$$K'_T = \frac{16}{9} \frac{P}{K_T} + \left(1 - \frac{4}{3} \frac{P}{K_T} \right) \left[\left(K'_0 - \frac{5}{3} \right) \left(\frac{V}{V_0} \right) + \frac{5}{3} \right] \quad (10)$$

$$K'_T = (K'_0 + 1) \left(\frac{V}{V_0} \right) - 1 \quad (11)$$

3.5. Volume Thermal Expansion Coefficient

An important and classical constant is obtained when the volumetric thermal expansion coefficient is applied to the isothermal bulk modulus. This principle has been widely studied in the field of materials science and its credibility and applicability has been greatly verified [35]. Such discoveries not only further our theoretical and experimental knowledge base, they also significantly extend the application of materials science to various fields and technologies [35].

$$\alpha_v K_T = \text{constant} \quad (12)$$

The below relations was demonstrated in the literature [35]: relation:

$$\alpha_v K_T = \alpha_{v0} K_0 \quad (13)$$

$$\alpha_v = \alpha_{v0} \left(\frac{K_0}{K_T} \right) \quad (14)$$

3.6. Exploring the relationship between the Gruneisen parameter and its dependence on pressure and volume

The Grüneisen parameter is one of the most important parameters, but it also plays a crucial role in thermodynamic studies, especially in understanding how energy and volume behave in different environments. Examining its reliance on volume and pressure raises several theoretical dilemmas and experimental opportunities that are particularly intriguing. This aspect of the problem remains poorly studied because of the limits on the existing theoretical frameworks and the sparsity of experimental data. Simply put, the pursuit of the

Grüneisen parameter under this challenge should be one such advancement in theory, as it would deepen our understanding of thermodynamics over the next several years and thus inform future methods and applications in the field [36]. Borton-Stacey formula reliably calculates the Gruneisen parameter under high compression conditions as mentioned below:

$$\gamma = \gamma_0 \left(1 + \frac{K'_0}{K_0} P \right)^{-1} \quad (15)$$

3.7. Compression-dependent Debye temperature

The Debye temperature (θ_d), which varies with pressure can be articulated as follows [37]:

$$\theta_d = \theta_0 \left(\frac{V}{V_0} \right)^{-\gamma} \quad (16)$$

It is beneficial to utilize Equations (14), (15), and (16) to ascertain key thermophysical properties of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$, specifically the pressure-dependent volumetric thermal expansion coefficient, Grüneisen parameter, and Debye temperature. Among these, the Debye temperature is particularly significant, as it marks the point at which the specific heat capacity transitions from temperature-independent to temperature-dependent behavior. This understanding enhances our insight into the material's thermal and mechanical responses, thereby facilitating improved control over the performance of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. The input values of the bulk modulus $K_0 = 87.11$ GPa, and the pressure derivative of bulk modulus is $K'_0 = 4$ [38].

Figure 3 illustrates the relationship between pressure (P) and the normalized volume (V/V_0) of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. It compares the output of several equations of state (EOS), in particular those used in Srivastava–Pandey, Brennan–Stacey and the Usual–Tait, and what DFT calculations and experimental results point to. That is the applied pressure, measured in gigapascals (GPa). As one would expect, all the curves slide down and on to the right, what might be called a decline in volume with increased pressure, something that happens to solids which are squeezed under pressure. Thus, we assume that each curve follows a nearly straight path, resulting in a much more consistent compression along the way. Even under such pressures, DFT and experimental analysis are in good agreement. For myself, this means DFT methods can correctly represent how the material pressure changes. On the other hand, the Srivastava-Pandey and Usual-Tait EOS models predict a stiffer material and the Brennan-Stacey EOS models are less rigorous and predict lower pressures. Overall, all the model correlations are quite good and perform as expected, thus confirming these EOS equations for mechanics in the case of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ is squeezed.

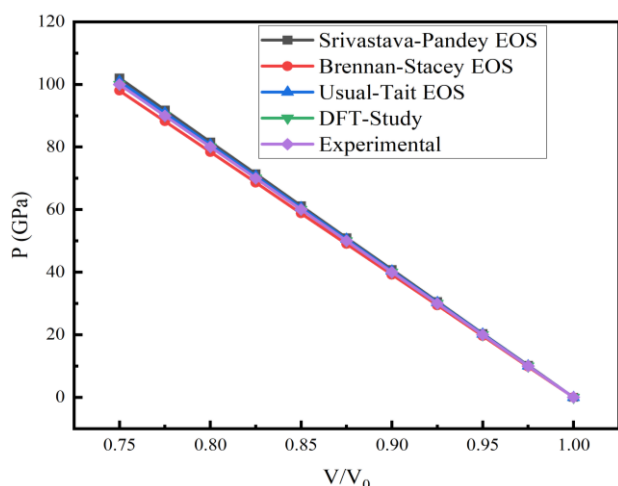


Fig. 3. Variation of pressure with compression $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.

As the same parameters are being predicted with the same agreement, the success of DFT methods and phenomenological methods of EOS in describing pressure-induced volume changes is confirmed. $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ will eventually compress in a predictable way and we cannot go on ignoring this in order to assess the structural alteration of this material. We suspect that the result of this observation may offer some tools for high-pressure superconducting or electronic systems.

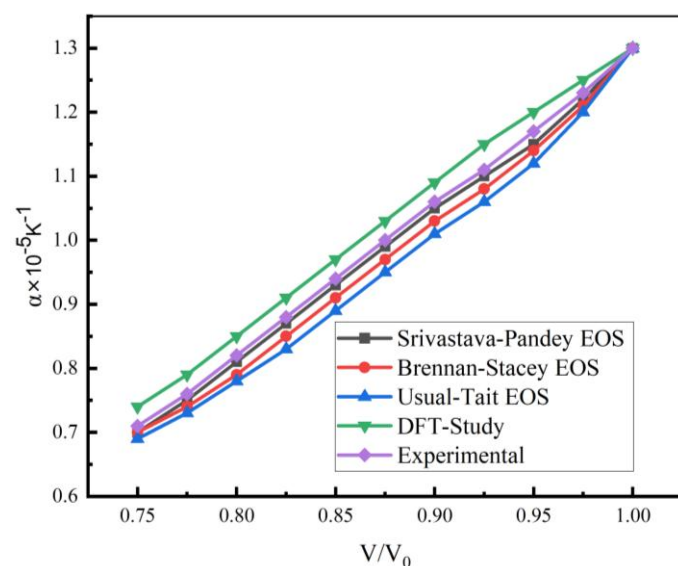


Fig. 4. Variation of volume thermal expansion coefficient with compression $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.

Now, as you squeeze $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ to reduce the normalized volume value, V/V_0 , the thermal expansion coefficient, α , of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ is also lowered (Figure 4). From these DFT calculations, experimental data, and these

three different EOS as presented, Srivastava–Pandey’s one, Brennan–Stacey’s one, and Usual–Tait’s one, it seems they will perform equally well and compared to us here. Essentially, it was expected that higher pressure and lower V/V_0 would lead to a decrease in thermal expansion. This makes perfect sense: atoms that have been squashed don’t vibrate as readily, and that’s why expansion slows. Below about equilibrium pressure, typically around 1 V/V_0 (normal pressure), α is elevated to about $1.3 \times 10^{-5} \text{ K}^{-1}$. By now, since V/V_0 now declines to approximately 0.75, α approaches $0.7 \times 10^{-5} \text{ K}^{-1}$. Although the DFT calculations compare slightly to the EOS models, they come out perfectly in agreement with the experimental data, which is very encouraging. Srivastava-Pandey and Brennan-Stacey EOS models provide a similar α for the middle ground. In contrast, the Usual-Tait EOS yields slightly smaller α values at any pressure level. Punch it down, and the thermal expansion becomes stifled. That DFT, the EOS, and experimentation all appear to agree so nicely is a useful reminder that we can trust these metrics for representing the behaviors of materials exposed to extreme pressure and temperature conditions, which, if anyone wants to establish their stability and performance in extreme environmental conditions, cannot be more obvious.

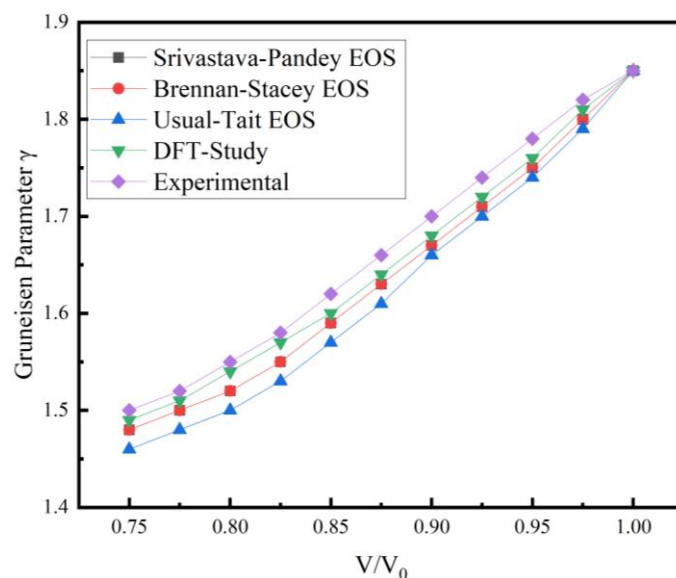


Fig. 5. Variation of Gruneisen parameter with compression $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.

The calculations of the Gruneisen parameter by DFT and three equations of state, such as the Srivastava–Pandey equation, the Brennan–Stacey equation, and the standard Tait equation of state (EOS), are compared in Figure 5 for $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. One exciting aspect is that the Gruneisen parameter increases with volume, so it decreases with pressure. This makes physical sense because crystalline solids get a little wonky (anharmonic) at lower pressure. At standard pressure ($V/V_0 = 1$), γ is elevated to a maximum

value, approximately 1.85. Then it gradually collapses to around 1.45 when the volume drops to 0.75 V_0 . Thus, greater mechanical pressure compressions and decreased anharmonic changes with increasing material pressure reduce the effect of vibrations. At present, all of these curves do something similar, although with some subtle variations.

The Srivastava–Pandey & Brennan–Stacey EOS models yield somewhat higher values than the Tait EOS, where the same volumes predict similar but slightly lower γ values. So they're all in the same ballpark, generally this is good for explaining γ change with pressure when used with this material. On balance, these numbers imply that anharmonic effects decrease with increasing pressure. These DFT and EOS models illustrate clearly and conform to the real-world phenomena. As such, it is significant for predicting several features, for example, thermal conductivity, phonon-limited scattering, and heat capacity, enabling accurate prediction as pressure is applied in designing for specific properties, and then we can modulate electronic and thermal properties.

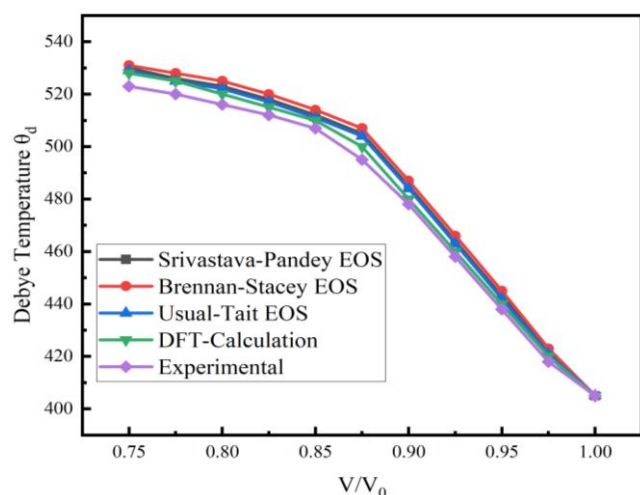


Fig. 6. Variation of Debye temperature with compression $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$.

Examine Figure 6, we can see how the Debye temperature (θ_d) changes with the normalized volume (V/V_0) for $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. As shown in Figure 5, this section compares DFT calculations and experimental results with three equations of state (EOS): Srivastava–Pandey, Brennan–Stacey, and the Usual–Tait equation. On the x-axis, the relative volume V/V_0 decreases with increasing compression. At the same time, on the y-axis, the Debye temperature is given in Kelvin and is essential for material thermal and vibrational properties. First, at decreased volume (pressures), the Debye temperature increases. Then, starting from approximately 405 K at normal pressure $V/V_0=1$, it goes up to 530–540 K at about 0.75 V/V_0 . This means that when the material is squeezed, phonon frequencies increase because the lattice becomes stiffer. The atoms will be closer to each

other; thus, the interatomic forces increase and rise as the vibrational energy increases [39].

All the curves line up reasonably well, though one or two differ slightly between the models. It seems the Brennan–Stacey EOS overestimates the Debye temperature at higher pressures. The experimental curve is slightly below the DFT and EOS predictions, so the readings are somewhat underestimated. However, these differences are pretty minor, and the models all agree reasonably well, so it is possible to validate the theory both in the experimental work and in the models. Thus, the figure shows that, with increasing pressure, the Debye temperature rises, indicating an increase in the vibrational strength in $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. The high agreement among DFT, experimental values, and EOS models suggests that all three methods are the most consistent and reliable for studying changes in thermal behavior under pressure. The nature of this information, essential for determining lattice stability, how much heat it retains, and, under high pressure, the movement of phonons, is necessary for materials that can be useful in thermoelectric and superconducting applications.

4. CONCLUSION

In this work we set out to understand how applied pressure modifies the structural, mechanical, and thermal behavior of the high temperature superconductor $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$. Using density functional theory together with carefully chosen computational parameters, we simulated hydrostatic compression up to 100 GPa and compared our results with available experimental data and several equations of state. One of the clearest findings is the strongly anisotropic compression pattern. The c axis shrinks far more than the a axis under pressure, and this observation aligns perfectly with the layered perovskite type structure where strong covalent bonding within the CuO_2 planes resists in plane compression while weaker interlayer forces allow the out of plane direction to collapse more easily. The elastic constants we computed increase monotonically with pressure, and all of them satisfy the stability criteria, which means the material does not undergo any mechanical instability in this pressure range. The steady rise in bulk modulus, shear modulus, and Young's modulus all point toward a systematic stiffening effect. When we turned our attention to thermal properties, the Debye temperature increased noticeably with compression, reflecting a hardening of the phonon modes. At the same time, both the Grüneisen parameter and the volume thermal expansion coefficient decreased, indicating that anharmonic effects become less significant as the lattice is squeezed. What makes these results practically useful is the excellent consistency between our DFT predictions, the experimental benchmarks, and the various equation of state models. This agreement tells us that the computational approach we used is trustworthy and can be extended to other layered cuprates. Overall, $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ emerges as a material that remains mechanically robust under extreme pressures while showing a clear and predictable evolution of

its thermal properties. These insights should help guide future efforts to design or optimize superconductors for applications that involve high pressure environments.

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

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Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Author's contribution statement

Dr. Abhay Prakash Srivastava prepares a preliminary version of the manuscript under the guidance of Dr. Brijesh Kumar Pandey.

Data availability statement

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

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