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Lattice Mechanical Properties of Alkaline Earth Metals Calcium and Strontium

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Application of pseudopotential theory is challenging in the theoretical study of lattice mechanical properties of heavy alkaline earth metals, in which sp-d hybridization plays an important role as d-bands of these metals are very close to Fermi level. A local form of the pseudopotential due to George et al. has been used in the present study to compute the equilibrium lattice constant (R_0), binding energy (E), phonon dispersion curves in symmetry directions, interatomic potential ($V(r)$), mode Gruneisen parameter ($\gamma(q,j)$), dynamical elastic constants (C_{11}, C_{12} C_{44}), shear modulus (C'), bulk modulus (B), phonon density of states ($g(\upsilon)$), specific heat at constant pressure (C_P), isothermal bulk modulus (B_T), Debye Waller factor (W_T), mean square displacement ($\overline{U^2}$), Debye temperature (θ_D), Cauchy ratio ($\frac{C_{12}}{C_{44}}$), Poisson ratio (σ), Young's modulus (Y) and propagation velocities of elastic waves in symmetry directions of alkaline earth metals Ca and Sr. Computed results of these physical properties are compared with available experimental results and found to be in good agreement. Such capability of presently used local pseudopotential suggests that the pseudopotential itself accounts s-p-d hybridization in alkaline earth metals Ca and Sr without introducing a short range Born-Mayer like repulsive potential.

Keywords: Pseudopotential, Alkaline earth metals, Lattice dynamics, Lattice mechanical properties.

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1. INTRODUCTION

In alkaline earth metals Ca and Sr, the presence of nearly empty d-band in the close proximity to *s-p* band near Fermi level makes their electronic structure complicated as conduction electrons have some *d*-like character [1, 2]. Thus, free electron theory is not capable to fully describe properties of these metals as *sp-d* hybridization plays an important role in the description of behavior of these metals, which are found to be in fcc structure at zero temperature and pressure [1-4]. Pseudopotential theory, due to its computational simplicity, is found to be successful in the study of static, thermodynamic, and many other physical properties of different class of metals [1-7]. The study of phonon spectra and other lattice mechanical properties gives satisfactory description of interatomic interactions persisting in the metals. In the present study, we have carried out study of some static and lattice mechanical properties of fcc calcium and fcc strontium using local pseudopotential [8]. The physical properties studied in the present communication are volume variation of binding energy, equilibrium lattice constant (R_0) and binding energy (E), phonon dispersion curves, inter-atomic potential $V(r)$, mode Gruneisen parameter ($\gamma(q,j)$), dynamical elastic constants (C_{11}, C_{12}, C_{44}), shear modulus (C'), bulk modulus (B), phonon density of states ($g(\upsilon)$), Cauchy ratio ($\frac{C_{12}}{C_{44}}$), Poisson ratio (σ), Young's modulus (Y) and propagation velocities of elastic waves in symmetry directions along with temperature variation of specific heat at constant pressure (C_P), isothermal bulk modulus (B_T), Debye Waller factor (W_T), mean square displacement ($\overline{U^2}$) and Debye temperature (θ_D).

2. THEORY

The pseudopotential due to George *et al.* [8] has the following form in q-space

$$V_{ion}(q) = \frac{1}{\Omega}\left[-\frac{8\pi Z}{q^2} + \beta exp(-q^2 {r_c}^2)\right]. \tag{1}$$

Here, β and r_c are two adjustable pseudopotential parameters. Z and Ω are the valence and atomic volume, respectively. The Hartree dielectric function along with exchange and correlation function due to Hubbard and Sham [9-11] has been used in the present study to find screened form factor.

Binding energy or cold energy E is a sum of electron gas energy E_{eg}, the first order correction to the energy E_1, the electrostatic energy E_{es} and the band structure energy E_{bs} [7]

$$E = E_{eg} + E_1 + E_{es} + E_{bs}. \tag{2}$$

Equation (2) was used to determine the pseudopotential parameters β and r_c by minimizing binding energy E at normal volume (zero pressure condition) without favoring any other physical quantity.

In the present study, the methods described in [12] have been used to calculate the lattice mechanical properties, and relevant expressions of these physical properties have also been taken from [12].

3. RESULTS AND DISCUSSION

Different sets of pseudopotential parameters were determined by using zero pressure condition. The set of parameters, which gives overall good results of both phonon dispersion curves and binding energy at zero pressure, was selected. The pseudopotential parameters and other input parameters used in the present study are tabulated in Table 1.

Table 1 – Pseudopotential parameters along with other input parameters

Metal	Z [1]	Ω (a.u.^{3})	M (amu)	R_C (a.u.)	β
Ca	2	293.5 [13]	40.078 [14]	0.8	80
Sr	2	373.6 [1]	87.62 [14]	0.9	108

3.1 Binding Energy

Binding energies of Ca and Sr as a function of lattice constant and hence volume are shown in Fig. 1. Minima of these curves give the equilibrium binding energy and lattice constant, which are tabulated in Table 2 along with experimental and other theoretical results.

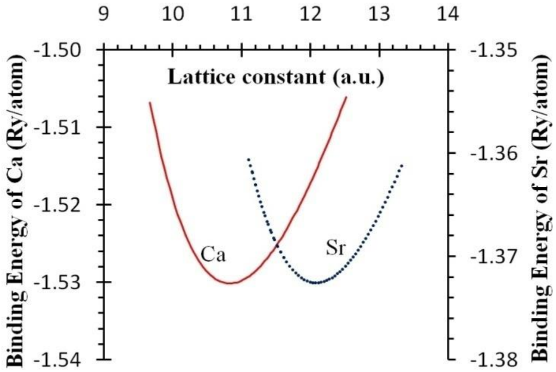

Fig. 1 – Solid and dotted lines represent binding energies of Ca and Sr, respectively, as a function of lattice constant

Binding energies of Ca and Sr are found to be in good agreement with experimental results with 5.01 and 1.24 % variations, respectively. Presently obtained lattice constants of Ca and Sr are also found to be in good agreement with the experimental results with 2.60 and 5.62 % variations, respectively. Superscripts *a, b, c, d* and *e* represent different models used by Moriarty [1] in his study. Superscripts *f* and *g* represent *rev PBE vdW* and *PAW GGA* used in the study of Park *et al.* [15]. Presently computed results of binding energy and lattice constants are also found to be in good agreement with other theoretical results.

Table 2 – Binding energy ($-E$) and lattice constant (R_0) of Ca and Sr

Metal	Lattice constant (a. u.)			Binding energy (Ry/atom)		
	Present	Exp.	Others	Present	Exp.	Others
Ca	10.823	10.549 [13]	10.498[15], 10.457[15], 10.7243[3]	1.530	1.457 [1]	1.361[1], 1.270[1], 1.347[1], 1.373[1], 1.378[1], 1.442[15], 1.462[15], 1.48424[3]
Sr	12.075	11.433 [1]	11.449[15], 11.3913[15], 11.69905[4]	1.372	1.355 [1]	1.206[1], 0.528[1], 1.093[1], 1.118[1], 1.200[1], 1.330[15], 1.348[15], 1.376187[4]

3.2 Phonon Dispersion Curves

Lattice mechanical and most of thermal properties of metals can be described by knowing phonon frequencies. The phonon dispersion curves in major symmetry directions are obtained by diagonalizing the matrix elements. Phonon dispersion curves of Ca and Sr along with experimental results [16, 17] are displayed in Fig. 2.

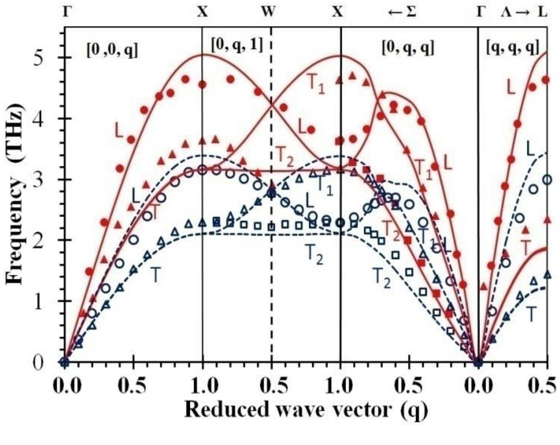

Fig. 2 – Solid lines and broken lines represent phonon dispersion curves of Ca and Sr, respectively, in symmetry directions. Experimental points for Ca (solid points) and Sr (hollow points) are due to Stassis et al. [16] and Buchenau et al. [17], respectively

It is evident from Fig. 2 that the pseudopotential used in the present study reproduces the phonon frequencies in overall good agreement with the experimental results. It is important to point out that the pseudopotential parameters were not obtained by fitting the phonon frequency at zone boundary. In order to use the model potential for the comprehensive study of physical properties, pseudopotential parameters should be determined using zero pressure condition. In this sense, the overall good agreement of phonon frequencies with the experimental results is remarkable achievement of the model.

3.3 Interatomic Potential

Interaction between ions is studied by knowing interatomic potential $V(r)$, which is required in the study of lattice defect calculations because exponential behavior at small atomic distance shows hard sphere like behavior [12]. Interatomic potentials of Ca and Sr are shown in Fig. 3. Minima of $V(r)$ for Ca and Sr are found at $r = 8.708\, a.u.$ and $r = 9.541\, a.u.$, respectively. The first nearest neighbor distances for Ca and Sr are 7.459 a.u. and 8.084 a.u., respectively, which are close to the value of r at minima of $V(r)$ for both metals.

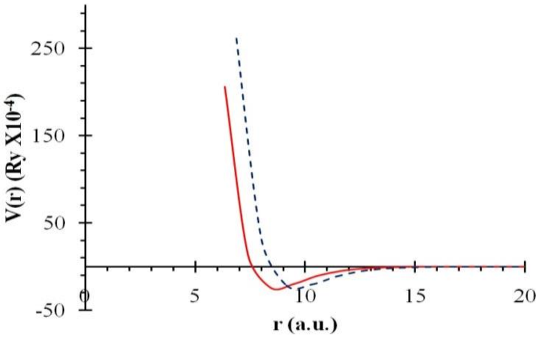

Fig. 3 – Solid line and broken line represent interatomic potential of Ca and Sr, respectively

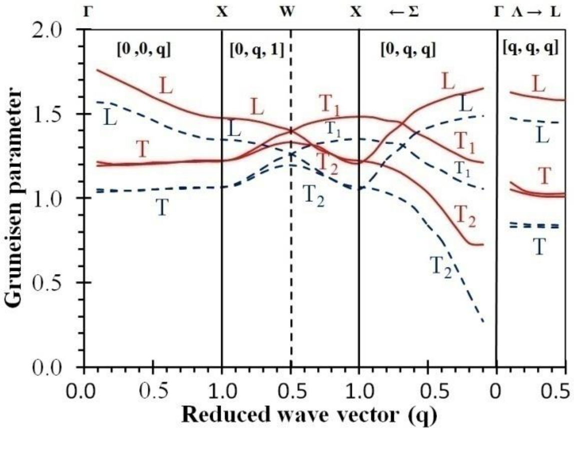

Fig. 4 – Solid and dotted lines represent mode Gruneisen parameter of Ca and Sr, respectively

3.4 Mode Gruneisen Parameter

The dependence of phonon frequency on volume and hence pressure is described by mode Gruneisen parameter which is defined as $\gamma(q,j) = \frac{-d[ln\omega(q,j)]}{d[ln\Omega]}$. Here, q is the wave vector, j is the branch index. Calculated results of mode Gruneisen parameter of Ca and Sr are represented in Fig. 4. The reliability of a lattice dynamical model can be tested by comparing the computed results with experiment. Experimental study of mode Gruneisen parameter has not been reported in literature. The experimental studies of pressure dependence of phonon peaks were carried out by using tunneling spectroscopy [18, 19], which indicates that transverse modes are more sensitive to compression as compared to longitudinal ones. Computed results of γ_L for both metals are more than γ_T i.e longitudinal modes are sensitive to compression, and the experimental studies [18, 19] conclude that such metals have no phonon anomalies. It is also concluded from experimental study that transverse modes are more sensitive to longitudinal modes for metals having phonon anomalies [18, 19].

3.5 Dynamical Elastic Constants

Dynamical elastic constants (C_{11}, C_{12}, C_{44}) have been calculated using expressions in terms of tensor force constants (see Ref. [12]). Shear modulus C' and bulk modulus B have also been calculated. Calculated results of C_{11}, C_{12}, C_{44}, C' and B are compared in Table 3 with experimental and other theoretical results. Results of C_{11}, C_{12}, C_{44}, C' and B of Ca are in good agreement with available experimental and other theoretical results. Results of C_{12}, C_{44}, and C' of Sr are not as good as results of Ca.

Table 3 – Dynamical elastic constants (C_{11}, C_{12} and C_{44}), shear modulus (C') and bulk modulus (B) for Ca and Sr. All quantities are in 10^{12} dyne/cm^2

	Ca			**Sr**		
	Present	**Experimental**	**Others**	**Present**	**Experimental**	**Others**
C_{11}	0.279	0.27801 [16]	0.1863 [21]	0.268	0.17 [17]	0.1888 [21]
C_{12}	0.145	0.18225 [16]	0.1771 [21]	0.136	0.1204 [17]	0.1473 [21]
C_{44}	0.155	0.16304 [16]	0.1509 [21], 0.1704 [20]	0.145	0.099 [17]	0.1180 [21]
C'	0.067	0.04788 [16]	0.0046 [21], 0.0523 [20]	0.0664	0.0248 [17]	0.02075 [21]
B	0.190	0.187 [20]	0.1802 [21], 0.1968 [20]	0.1801	0.1369 [17]	0.161 [21]

3.6 Phonon Density of States

Phonon density of states or phonon frequency distribution curve is required to study Debye temperature as a function of temperature [12]. Phonon densities of states for Ca and Sr are shown in Fig. 5.

3.7 Specific Heat

Specific heat at constant pressure (C_P) for Ca and Sr along with available experimental and other theoretical results are shown in Fig. 6. Presently calculated result of C_P of Ca has maximum deviation of 5.60 % from experimental results [22] near 300 K (see Fig. 6). Maximum deviation of 8.98 % is found between presently obtained result of C_P of Sr and theoretical result [23] near 300 K (see Fig. 6).

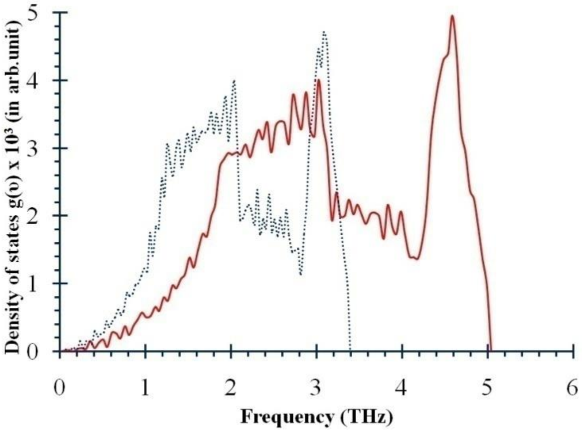

Fig. 5 – Solid and dotted lines represent phonon density of states of Ca and Sr, respectively

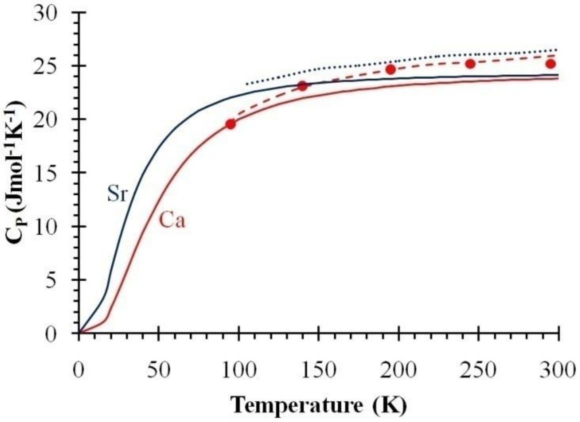

Fig. 6 – Specific heat at constant pressure (C_P) of Ca and Sr as a function of temperature. Experimental points of Ca are due to Hultgren et al. [22], which have been taken from Ref. [23]. Broken and dotted lines represent theoretical results [23] of Ca and Sr, respectively

3.8 Isothermal Bulk Modulus

Presently calculated results of isothermal bulk modulus B_T of Ca and Sr are displayed in Fig. 7 and are found to be in good agreement with theoretical results due to MacDonald and MacDonald [23] (not shown in Fig. 7). Maximum variation of 9.62 % is found at 100 K between presently calculated results of B_T and results due to MacDonald and MacDonald [23] for Ca. In the case of Sr, maximum variation between presently calculated results of B_T and results due to MacDonald and MacDonald [23] is 16.93 % at 300 K.

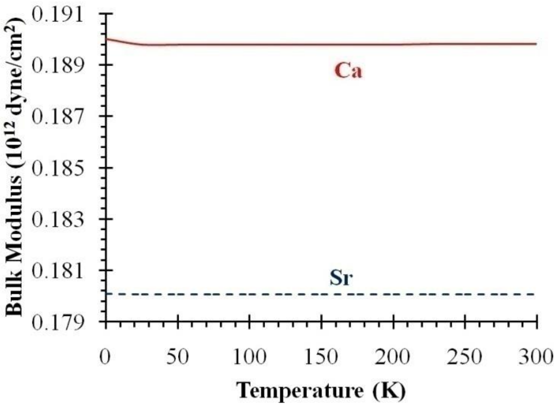

Fig. 7 – Isothermal bulk moduli of Ca and Sr as a function of temperature

3.9 Debye Waller Factor and Mean Square Displacement

The results of Debye Waller factor W_T and mean square displacement $\overline{U^2}$ of Ca and Sr are shown in Fig. 8 and Fig. 9, respectively, along with the experimental results [24]. Experimental results of mean square displacement ($\overline{U^2}$) have been calculated from the results of Debye Waller factor (W_T).

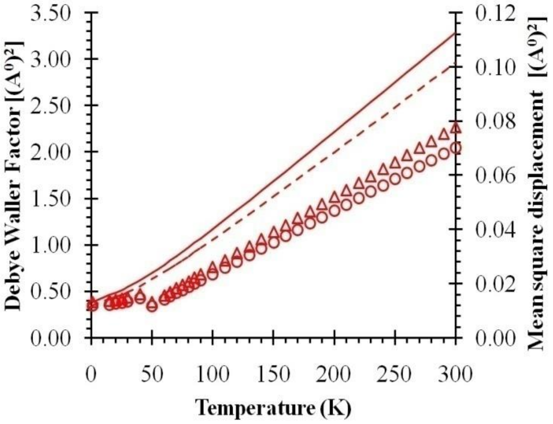

Fig. 8 – Debye Waller factor and mean square displacement of Ca along with experimental results [24]. Solid and broken lines represent presently computed results of mean square displacement and the Debye Waller factor, respectively. Triangles and circles represent experimental results [24] of mean square displacement and the Debye Waller factor, respectively

3.10 Debye Temperature

Debye temperature θ_D is an important physical property of material, which is associated with vibrational behavior of the material. Thus, physical properties, like specific heat, vibrational entropy and thermal expansion, can be described by θ_D [12]. Debye

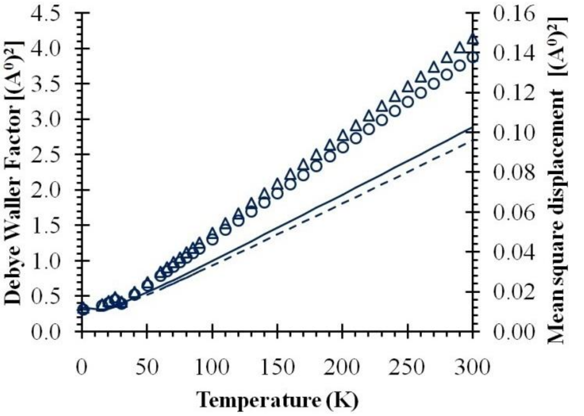

Fig. 9 – Debye Waller factor and mean square displacement of Sr along with experimental results [24]. Solid and broken lines represent presently computed results of mean square displacement and the Debye Waller factor, respectively. Triangles and circles represent experimental results [24] of mean square displacement and the Debye Waller factor, respectively

temperatures of Ca and Sr as a function of temperature are shown in Fig. 10. Results of θ_D of Ca are in good agreement with the experimental results [16] as variation of present result with experimental result is less than 4.00 % above 80 K. Maximum variation of 11.78 % is observed at 20 K between present result and experimental result of θ_D of Ca. We could not compare results of θ_D of Sr due to unavailability of experimental or other theoretical results.

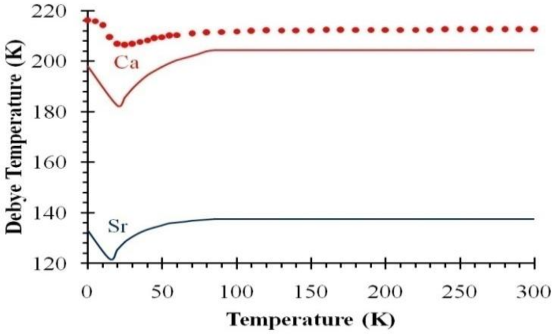

Fig. 10 – Debye temperature of Ca and Sr as a function of temperature. Experimental points of Ca are due to Ref. [16]

3.11 Cauchy Ratio, Poisson Ratio, Young's Modulus and Propagation Velocities of Elastic Waves

Volume dependent terms in the energy are an important factor in the description of longitudinal elastic constants C_{11} and C_{12}. But transverse elastic constant C_{44} has no such contributions, and the difference between C_{11} and C_{12} is proportional to C_{44}. The Cauchy's relation will be satisfied due to the volume independent term, which will lead to equilibrium under two-body central force. However, experimentally it is observed that Cauchy's relation is not satisfied by any metal. It is due to the volume dependence of the effective interaction [12]. The Cauchy ratio $\frac{C_{12}}{C_{44}}$, the Poisson ratio $\sigma = \frac{C_{12}}{[C_{11}+C_{12}]}$ and the Young's modulus $Y = 3B[1-2\sigma]$ have been computed in the present study. The vibration in the crystals leads to acoustic waves in the crystal, which are used to study lattice defects, electronic structure and many other physical properties of the crystal. The propagation velocities of longitudinal and transverse waves in symmetry directions have been calculated as (see Ref. [12]) $V_L[100] = \left[\frac{C_{11}}{\rho}\right]^{1/2}$; $V_T[100] = \left[\frac{C_{44}}{\rho}\right]^{1/2}$; $V_L[110] = \left[\frac{C_{11}+C_{12}+2C_{44}}{\rho}\right]^{1/2}$; $V_{T1}[110] = \left[\frac{C_{44}}{\rho}\right]^{1/2}$; $V_{T2}[110] = \left[\frac{C_{11}-C_{12}}{2\rho}\right]^{1/2}$; $V_L[111] = \left[\frac{C_{11}+2C_{12}+4C_{44}}{3\rho}\right]^{1/2}$; and $V_T[111] = \left[\frac{C_{11}-C_{12}+C_{44}}{3\rho}\right]^{1/2}$. Here ρ is the density of the crystal. Cauchy's ratio $\frac{C_{12}}{C_{44}}$, Poisson's ratio σ, Young's modulus Y and propagation velocities of elastic waves for Ca and Sr are tabulated in Table 4 along with experimental results. Experimental results in Table 4 have been calculated by using experimental values of C_{11}, C_{12}, C_{44} (see Table 3) and ρ which is obtained using the experimental value of the lattice constant (Table 2). For present results of propagation velocities, ρ has been obtained by using our calculated lattice constant (see Table 2). Computed results of $V_L[100]$, $V_T[100]$, $V_L[110]$, $V_{T1}[110]$ and $V_L[111]$ of Ca are in excellent agreement with the experimental results as variation of present results with the experimental results is less than 5.00 %. Calculated results of C_{12}/C_{44}, σ and $V_T[111]$ of Ca differ by less than 17.00 %, while $V_{T2}[110]$ by 23.08 % with the experimental results. Calculated results of Y of Ca do not agree well with the experimental results. Calculated results of C_{12}/C_{44}, σ, $V_L[100]$, $V_T[100]$, $V_L[110]$ and $V_{T1}[110]$ of Sr are in reasonably good agreement with the experimental results while the results of Y, $V_{T2}[110]$, $V_L[111]$ and $V_T[111]$ do not agree well with experimental results.

Table 4 – Cauchy ratio, Poisson ratio, Young's modulus (in 10^{12} dyne/cm^2) and propagation velocities (in 10^5 cm/s) of elastic waves in Ca and Sr

	Ca		**Sr**	
	Present	**Exp. [16]**	**Present**	**Exp. [17]**
C_{12}/C_{44}	0.935	1.118	0.938	1.216
σ	0.342	0.396	0.336	0.415
Y	0.180	0.117	0.177	0.070
$V_L[100]$	4.438	4.261	3.468	2.542
$V_T[100]$	3.306	3.263	2.547	1.940
$V_L[110]$	7.195	7.166	5.576	4.309
$V_{T1}[110]$	3.306	3.263	2.547	1.940
$V_{T2}[110]$	2.176	1.768	1.724	0.971
$V_L[111]$	5.287	5.309	4.089	3.198
$V_T[111]$	2.608	2.374	2.036	1.372

4. CONCLUSIONS

It is well-known fact that heavy alkaline earth metals behave like early transition metals due to the presence of empty d band very close to the Fermi level. Behavior of these metals is somehow intermediate between simple and transition metals. In order to account such complex electronic structure of these metals, in the present study, we have used a local form of the pseudopotential to study the lattice mechanical properties of Ca and Sr. Presently used pseudopotential has only two adjustable parameters, which are obtained by applying zero pressure condition instead of fitting experimental phonon frequencies at symmetry points. The pseudopotential is found to be successful in reproducing the lattice mechanical properties of Ca and Sr. Results obtained in the present study are in good agreement with the experimental and other theoretical results obtained by more sophisticated and first principle methods. Actually, first principle methods are more accurate and reliable, but are computationally expensive and complicated as those methods based on some well-known approximations, which require lengthy calculations. As an alternate method, we have used pseudopotential method, which is simple and easy to implement for computing. Such success of the presently used pseudopotential suggests that the sp-d hybridization and overlap effects in these metals are properly accounted by the pseudopotential itself without using any additional empirical Born Mayer type repulsive potential. It is also important to point out that actual valence has been used in the present study during determination of pseudopotential parameters and computation of the physical properties of Ca and Sr. It is concluded that effective valence is not required to fully describe the physical properties of early transition metals Ca and Sr and hence it is worthwhile to extend this pseudopotential for the study of physical properties of transition metals. Such studies are in progress and results are quite encouraging.

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Механічні властивості ґраток лужноземельних металів кальцію і стронцію

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Застосування теорії псевдопотенціалів є складним завданням у теоретичному дослідженні механічних властивостей ґратки важких лужноземельних металів, в яких sp-d гібридизація відіграє важливу роль, оскільки d-смуги цих металів дуже близькі до рівня Фермі. Локальна форма псевдопотенціалу (George et al.) була використана у даному дослідженні для розрахунку рівноважної постійної ґратки, енергії зв'язку, кривих дисперсії фононів у напрямках симетрії, міжатомного потенціалу, параметра Грюнайзена, динамічних пружних констант, модуля зсуву, об'емного модуля, фононної щільності станів, питомої теплоти при постійному тиску, ізотермічного модуля об'ємності, фактору Дебая-Валлера, середньоквадратичного зміщення, температури Дебая, коефіцієнта Коші, коефіцієнта Пуассона, модуля Юнга і швидкості поширення пружної хвилі в напрямках симетрії лужноземельних металів Ca і Sr. Обчислені результати цих фізичних властивостей порівнюються з наявними експериментальними результатами і знаходяться у узгодженні. Така здатність використовуваного тут локального псевдопотенціалу свідчить про те, що псевдопотенціал сам по собі враховує *s-p-d* гібридизацію в лужноземельних металах Ca і Sr без введення короткодіючого відштовхуючого потенціалу Борна-Майєра.

Ключові слова: Псевдопотенціал, Лужноземельні метали, Динаміка ґратки, Механічні властивості ґратки.