

Cohesive, Thermal and Elastic Properties of Alkali Superoxides

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Abstract

We have applied an Extended Three Body Force Shell Model (ETSM) for investigating the cohesive, thermal and elastic properties such as cohesive energy(ϕ), molecular force constant(f), compressibility(β), Restrahlen frequency (ν_0), Debye temperature (θ_D), Gruneisen parameter (γ), second Gruneisen parameter (q), Moelwyn Hughes constants (F_1), and ratio of volume expansion coefficient (α) to volume specific heat (c_v) of alkali superoxide. We have also reported the Third order elastic constant's(TOECs), pressure and temperature derivatives of Second order elastic constant's(SOECs). Elastic constant variation and Specific heat curve of alkali superoxide are also reported on the paper. And, we could compare our result of specific heat curve with the experimental data. Our computed specific heat results follow the same trends of variation with corresponding experimental data. The values of specific heats also increase with temperature. Our calculated results on specific heat are in closer agreement with the experimental data. Here, we could compare our result of cohesive, thermal and elastic properties with other available experimental data at room temperature.

Keywords: Cohesive, Thermal, Elastic, Specific Heat.

1. INTRODUCTION

The coupling between atomic motions (phonons) and the molecular orientations (pseudospin) is responsible for the structural phase transition in various molecular crystals. Ionic molecular solids undergo a series of structural phase transitions and show anomalous thermoelastic properties, which are intimately connected, with the orientational, spin and orbital degrees of freedom of the ionic molecular species. Typical examples are alkali cyanides[1-7](MCN), superoxides[8, 9](MO₂), azides[10](MN₃), hydroxides[11](MOH) and nitrites[12](MNO₂) where M is an alkali ion. In this class cyanides are the simplest, the (CN⁻) molecular ion possessing only orientational degrees of freedom whereas the superoxides are perhaps the most complex, the O₂⁻ ion possessing all three, i.e.orientational, orbital and spin degrees of freedom. Alkali superoxides, with chemical formula XO₂, where X=Na, K, Rb and Cs, exhibit a wide variety of phenomena[13-15]which can be directly related to the properties of the superoxide ion O₂⁻. For example, these systems show a series of first-order phase transitions which involve rearrangement of the molecular axes of O₂⁻ ions and are in certain cases accompanied by a change in the symmetry of the unit cell. Sodium superoxide is unique among alkali superoxides and is known to exist in a number of different crystalline forms. The properties of sodium superoxide have been well studied experimentally [16-20]. At room temperature the crystal has an orientationally disordered cubic structure with a space group Fm3m in which the molecular anions are undergoing rotational diffusion. Upon cooling to about 230K, an orientational ordering transition occurs. The crystal then adopts the cubic Pa3 (ordered pyrite) structure in which the molecular anions align along the body diagonals in a four sub lattice structure. Between 43K and 196K, NaO₂ is orthorhombic Pnmm (Marcasite structure) with the molecular anions now aligned along the unique axis.

In the heavier alkali- metal superoxides, the intermediate ordered pyrite phase is not observed, instead there is transition from the disordered pyrite phase directly to the marcasite phase. The nature of the interionic forces in NaO₂, and the factor that influence the relative stability of the ordered pyrite and marcasite phases, have been discussed by Mahanti and Kemeny[18]. It was concluded that electrostatic interactions, including the direct quadrupole- quadrupole interaction between the anions, favored pyrite phases whereas effects due to the crystal field and orbital degeneracy favored the marcasite phase[21]. The

order-disorder transition of the pyrite phases has been discussed using molecular-field approximation for the orientational degrees of freedom and ignoring the translational motion of the cations and anions the role of indirect interactions between the O_2^- ions, due to translational-rotational coupling[22]. For example these systems show a series of first-order phase transition which involve rearrangement of molecular axis of O_2^- ions and are in certain cases accompanied by change in the symmetry of the unit cell as shown in crystal structure.

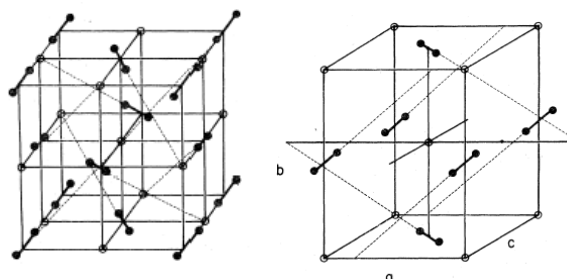


Fig. 1. Various structures of NaO_2 –(a) Ordered Pyrite and (b) Marcasite. The open circles represents the Na^+ ions, rest is O_2^- ions.

The special interest in sodium superoxide lies in the fact that it exhibits the NaCl structure, and has the lattice constant $a=5.64\text{\AA}$, very similar to that of NaO_2 , and the mass of chlorine is only about 10% heavier than that of O_2 .

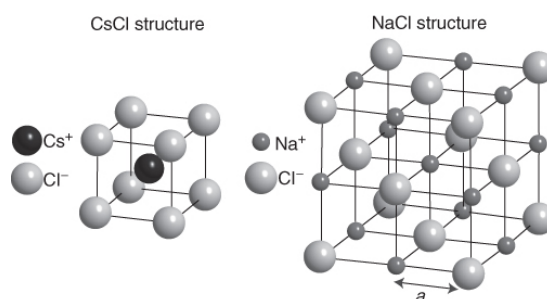


Fig. 2. Structure of NaCl and CsCl

Potassium superoxide has a face-centered tetragonal CaC_2 structure, which can be pictured as a NaCl arrangement with the O_2^- at Cl positions and with the molecular axis along the tetragonal axis[23]. Above 395K, KO_2 was found to possess a disordered cubic structure similar to the high temperature forms of NaO_2 . The lattice constant are $a=5.70(6.00, 6.28)\text{\AA}$ for $KO_2(RbO_2, CsO_2)$. In contrast, NaO_2 crystallizes in a cubic pyrite structure ($a=5.49\text{\AA}$) with rotationally disordered O_2^- groups. In NaO_2 the nearest neighbour distance is 2.73\AA whereas in KO_2 it is given as 2.55\AA . The Schematic diagram of KO_2 is given in Figure 3.

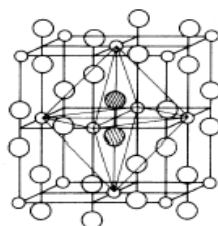


Fig.3. Structure of KO_2

We have developed an Extended Three-Body Force Shell Model (ETSM), this model has successfully been applied to study the static, dynamic, dielectric, optical and anharmonic properties of pure ionic crystals, cyanides and alkali halide- cyanide

mixed crystals having NaCl and CsCl structure. Looking to the considerable success of the ETSM[24-37], we have applied the ETSM to calculate the cohesive, thermal and elastic properties of alkali superoxides.

The essential formulation of the present model is given in the next section and the results obtained by us are presented and discussed in the subsequent section.

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2. RELATED WORK

The interaction potential used to derive the framework of the present ETSM can be expressed as[38]

$$\phi = - \frac{e^2}{2} \sum_{kk'} Z_k Z_{k'} r_{kk'}^{-1} \left[1 + \sum_{kk'} f_k(r_{kk'}) \right] - \sum_{kk'} c_{kk'} r_{kk'}^{-6} - \sum_{kk'} d_{kk'} r_{kk'}^{-8} - b \sum_{kk'} \beta_{kk'} \cdot \exp \left\{ \frac{r_{kk'} + r_{kk'} - r_{kk'}}{\rho} \right\} \quad (1)$$

where the first two terms represent the long range Coloumb and Three Body Interaction[35] the third and fourth terms are the van der Waals (vdW) interaction due to dipole-dipole (d-d) and dipole-quadrupole (d-q) attractions, the fifth term represents the HafemeisterFlygare[36] type short- range overlap repulsion extended up to second neighbour ions, $\beta_{kk'}$ are the Pauling coefficient[37] given by[38]

Cohesive and Thermal properties: Cohesive energy (ϕ) of a material is a fundamental property, which tells us about the cohesion in the system. If the cohesion for the material is negative it means that the constituent atoms will gain energy by reacting to form a compound (solid or molecule). The binding energy in ionic crystals can be explained by calculating their cohesive energy from large number of interatomic interaction potentials. The details of these potentials have been reviewed earlier by[39, 40]. The other parameters like molecular force constant (f), compressibility (β), Restrahlen frequency (ν_0), Debye temperature (θ_D), Gruneisen parameter (γ), Moelwyn Hughes constants (F_1) and ratio of volume thermal expansion coefficient (α_v) to volume specific heat (C_v) which are directly derived from the cohesive energy $\phi(r)$ are computed on the lines of Singh and Gaur[37, 38]

Elastic properties: We have studied the anharmonic elastic properties by calculating Second Order Elastic Constants (SOECs), [30-32]as they provide physical insight into the nature of binding forces between the constituents of the crystal and are strongly related to other anharmonic properties, like thermal expansion, thermoelastic constants and thermal conductivity. The expression for these elastic constants of SOECs are given by[38, 41-45, 50]

3. METHODOLOGY

Using the input data given in Table 1 for fcc C_{60} [46, 47] we have calculated the model parameters listed in Table 2.

Table 1: Input data for NaO_2 and KO_2

Properties	NaO_2	KO_2
r_0 (Å)	2.75 ^a	3.08 ^e
c_{11} (10^{11} dyn/cm ²)	5.80 ^b	4.99 ^f
c_{12} (10^{11} dyn/cm ²)	4.50 ^b	4.29 ^f
c_{44} (10^{10} dyn/cm ²)	3.80 ^b	4.09 ^f
α_+	0.28 ^c	1.30 ^c
α_-	2.45 ^d	2.45 ^d
C	291.20 g	594.96 g
D	126.75 g	466.74 g

a-[18], b-[16], c-[48], d-[12], e-[49], f-[extrapolated values obtained from r_0 versus for superoxides], [Calculated from ref. [50]

Table2: Model parameters for NaO_2 and KO_2

Compound	r (Å)	ρ (Å)	b (10^{12} erg)	$f(r)$
NaO_2	2.74	0.218	0.76125	-

	7	0		0.0059
KO ₂	3.11	0.191	0.65732	-
	2	0		0.0021

4. RESULTS AND DISCUSSION

Results and discussion are given below in the next sections:

Lattice static properties: We have calculated the compressibility (β), molecular force constant (f), Reststrahlen frequency (ν_0), Debye temperature (θ_D), Gruneisen parameter (γ), second Gruneisen parameter (q), Moelwyn Hughes constants (F_1), ratio of volume expansion coefficient (α_v) to volume specific heat (c_v), which are directly derived from the cohesive energy ϕ (r).

Table 3 Cohesive and Thermal properties for NaO₂ and KO₂

NaO ₂		KO ₂		
T(K)	300	300 _{expt}	300	300 _{expt}
ϕ (eV)	-830.35	-799 ^h	-740.11	-741 ^h
β (10 ⁻¹² dynes ⁻¹ cm ²)	5.987	4.933 ⁱ	8.854	4.523 ⁱ
f (10 ⁴ dynes. Cm ⁻¹)	2.7523	3.345 ^j	2.109	4.085 ^j
ν_0 (THz)	5.611		4.911	
θ_D (K)	269.31		235.74	
α_v/c_v	4.193		4.227	
γ	2.440		3.130	
q	2.461		3.135	
F_1	5.629		6.667	

h-Ref. [52], i- $[\beta=3/(c_{11}+2c_{12})]$, j- $[f=3Kr_0/\beta]$

The Table 3 shows that our values on cohesive energy and compressibility (β) are in good agreement with their available data[51]. The other thermodynamic properties listed in table 3 could not be compared due to lack of experimental data.

Anharmonic elastic properties: Harmonic and anharmonic elastic constants at different temperatures are calculated by using the cohesive energy equation. The purpose of the study of elastic constant is to test mechanical stability of the potential.

In the following sections, we present our calculated results for the second order elastic constants as a function of temperature.

Using the model parameters, we have computed the second order elastic constants. While computing these constants, the translational-rotation coupling of the O₂ ion is taken into account. The TR coupling is incorporated on the lines of Sahu and Mahanti[53]. The calculated values of c_{11} , c_{12} and c_{44} at different temperature for NaO₂ and KO₂ are displayed in Figure 4.

The temperature dependent rotational susceptibility and anharmonicity are calculated on the lines of ref[54]. The temperature dependence of second order elastic constant is governed mainly by the short range repulsion and quadrupole contributions to the translational- rotational coupling. With the help of above equations, we have calculated SOECs for NaO₂ and KO₂ in the temperature range $50K \leq T \leq 450K$.

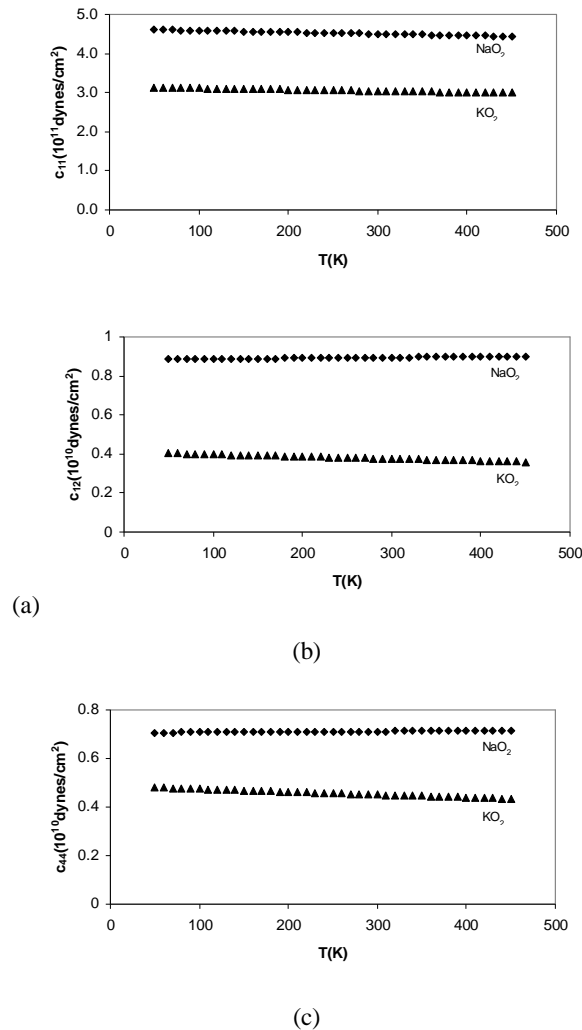


Fig. 4. Second Order Elastic Constants (a) c_{11} (b) c_{12} and (c) c_{44} as a function of temperature; square (■) and triangle (▲) represents the c_{ij} for NaO_2 and KO_2 respectively.

Here, we have investigated the effect of temperatures on elastic constants at $50\text{K} \leq T \leq 450\text{K}$. The major trend observed in the elastic constants decrease with increasing temperature. The magnitudes of SOECs seem to be correct. Also the ETSM method produces the sign of SOECs correctly.

Specific heat curve: We have reported the specific heat variation of NaO_2 and KO_2 within the temperature range $50\text{K} \leq T \leq 150\text{K}$ and shown in Fig. 1 along with experimental results[51]. Our computed of specific heat as a function of temperature follow the similar trend as experimentally observed curve. The specific heat in the normal state of the material is usually approximated by the contribution of the lattice and electronic specific heat. In our ETSM model calculation, we have considered only the lattice contribution, which causes the discrepancy from measured specific heat curve. On the basis of above discussions, it may be concluded that ETSM has successfully explained the cohesive and thermal properties of NaO_2 and KO_2 . The result on specific heat can further be improved by incorporating the electronic contribution in specific heat expression. Here, some of the results on thermal properties are at present of academic interest but they will serve as a guide to experimental worker in future.

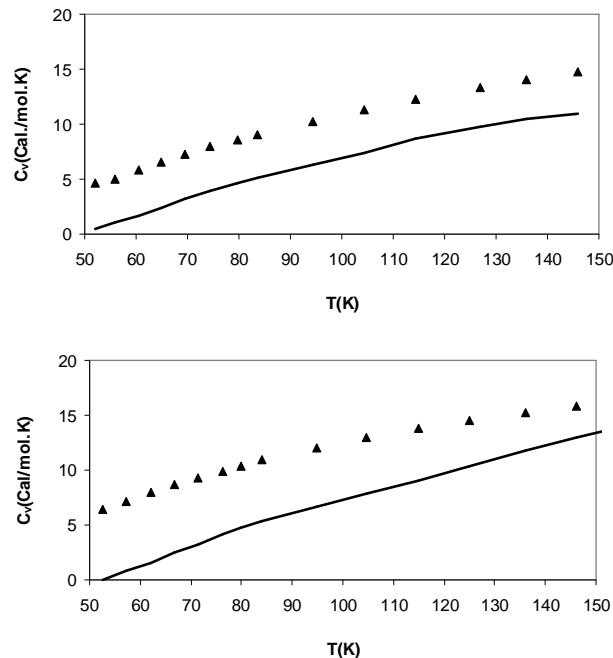


Figure 1: Variation of Specific heat of NaO₂ and KO₂ in the temperature ranges 50K ≤ T ≤ 150K. The solid line (—) and triangle (▲) are calculated and experimental data [51].

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