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Temperature Dependence of Anderson-Gruneisen Parameter for NaCl

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Abstract

Considering the thermodynamic and thermoelastic properties such as the volume thermal expansion, the thermal expansivity, the isothermal bulk modulus and the Anderson-Gruneisen parameter, we find that the already existed theories presented by other workers are imperfect for NaCl. In the present communication a new expression of temperature dependence of Anderson-Gruneisen has been constructed from room temperature to melting temperature. The results show good agreement with the experimental data.

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Keywords: Anderson-Gruneisen parameter, Thermal expansivity, Isothermal bulk modulus

1. Introduction

Various approaches for the determination of Anderson-Gruneisen parameter for NaCl has been discussed so far [K.Y.Singh, 2003; S.K.Srivastava, 2005; R.S.Chauhan, 2007; G.L.Cui, 2003; X.Q.Deng, 2002]. According to the definition

$$\delta_T = -\frac{1}{\alpha K_T}(\frac{\partial K_T}{\partial T})_P \tag{1}$$

One may easily obtain expressions of δ_T from the temperature dependence of thermal expansivity α and isothermal bulk modulus K_T.

Recently Singh and Chauhan [2002] have presented the following relationships

$$\alpha = \alpha_0[1 + c\alpha_0\delta_T^0(T - T_0)] \tag{2}$$

$$K_T = K_T^0[1 - d\alpha_0\delta_T^0(T - T_0)] \tag{3}$$

where c=1.35, d=1.06, and the subscript 0 in the equation of this paper denotes the reference value corresponding to every thermodynamic property at reference temperature $T_0 = 300K$. It's found that the results obtained from Eqs. (2) and (3) compare well with the experimental data [O.L.Anderson, 1995].

When substituting Eqs. (2) and (3) into Eq.(1), we can get the following Anderson-Gruneisen parameter

$$\delta_T = \frac{d\delta_T^0}{[1 + c\alpha_0\delta_T^0(T - T_0)][1 - d\alpha_0\delta_T^0(T - T_0)]} \tag{4}$$

On the other hand, Tallon [J.L.Tallon, 1980] found that the Anderson-Gruneisen parameter is directly proportional to the volume ratio V/V_0. Fang [2005] have got the following expressions for the temperature dependence of V/V_0 and the isothermal bulk modulus K_T for NaCl

$$\frac{V}{V_0} = 1 - \delta_T^0 \ln[1 - \alpha_0\delta_T^0(T - T_0)] \tag{5}$$

$$K_T = K_T^0[1 - \alpha_0\delta_T^0(T - T_0)] \tag{6}$$

Therefore the Anderson-Gruneisen parameter may be expressed as

$$\delta_T = \delta_T^0 \left\{1 - \delta_T^0 \ln[1 - \alpha_0 \delta_T^0 (T - T_0)]\right\} \tag{7}$$

Anderson [1995] has reported the experimental data of δ_T in the temperature range starting from room temperature up to 750*K*. Unfortunately, we find that both Eqs. (4) and (7) are inconsistent with the experimental data (see Fig.1).

The purpose of the present study is to determine a new expression of temperature dependence of Anderson-Gruneisen parameter for NaCl. We have compared the Anderson-Gruneisen parameter and the isothermal bulk modulus with other models. The method of analysis is shown in Section 2. The results are discussed in Section 3.

2. Method of Analysis

Anderson [1995] has reported accurate experimental data for the temperature dependence of Anderson-Gruneisen parameter δ_T for many solids. Analysis of the experimental data in the present work reveals that there exists a quadratic relationship between δ_T and temperature *T* for NaCl, which can be scripted as

$$\delta_T = \delta_T^0 [1 + b_1 (T - T_0) + b_2 (T - T_0)^2] \tag{8}$$

The values of b_1 and b_2 are obtained by fitting the experimental data on the Anderson-Gruneisen parameter at different temperatures. It has been found that $b_1 = 1.45 \times 10^{-4} K^{-1}$ and $b_2 = 5.40 \times 10^{-7} K^{-2}$.

Moreover, the above Eq. (2) has been found to be consistent with the experimental data on temperature dependence of thermal expansivity [O.L.Anderson, 1995]. Therefore, when combining Eqs. (2) and (8) with Eq.(1) , we get the following temperature dependence of the isothermal bulk modulus

$$K_T = K_T^0 \exp\left\{-\alpha_0 \delta_T^0 (T - T_0)[1 + c_1 (T - T_0) + c_2 (T - T_0)^2 + c_3 (T - T_0)^3]\right\} \tag{9}$$

Where $c_1 = (b_1 + c\alpha_0 \delta_T^0)/2, c_2 = (b_2 + cb_1 \alpha_0 \delta_T^0)/3$ and $c_3 = (cb_2 \alpha_0 \delta_T^0)/4$.

In order to test the validity of Eqs. (8) and (9) , we apply them to the experimental data. The corresponding curves are plotted in Figs. 1–2. The required parameters α_0, δ_T^0 and K_T^0 are $11.8 \times 10^{-5} K^{-1}$, 5.56 and 24GPa , respectively [O.L.Anderson, 1995].

3. Results and discussions

(1) Fig.1. shows that while discussing the Anderson-Gruneisen parameter for NaCl, Eq.(8) is the best among all the models. Although Singh and Chauhan [K.S.Singh, 2002] and Fang [Z.H.Fang, 2005] have made good attempts to study the thermodynamic properties such as volume thermal expansion, thermal expansivity and bulk modulus of NaCl, the relationships between the Anderson-Gruneisen parameter and temperatures derived from these theories deviate largely from the experiment. Hence, the conclusions made by Singh, Chauhan and Fang are imperfect.

(2) Anderson et al [O.L.Anderson, 1992] have assumed that the Anderson-Gruneisen parameter is a constant independent of temperature at a given pressure. It's noted that the last two terms in Eq.(8) can be neglected in the lower temperature range. But at high temperatures, they should be reserved. Therefore, assumption of constant Anderson-Gruneisen parameter is just applicable to low temperature regions near room temperature. At high temperature regions, the Anderson-Gruneisen parameter of NaCl should be expressed as Eq. (8).

(3) While the temperature is not too high, Eq. (9) changes directly into Eq. (6). But at high temperature regions, the last two terms in Eq. (9) must be retained, too. It's clear that predicted values of Eq. (9) show good agreement with the experiment (Fig.2).

4. Conclusion

We conclude that at temperature regions from room temperature to near melting temperature, the model proposed in the present study is superior to the other models. Eqs. (2), (8) and (9) constitute integrated thermodynamic and thermoelastic theories and can be used to understand the high-temperature behavior of NaCl.

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References

G.L.Cui, L.R.Chen. (2003). *Phys. Stat. Sol*., (b) 237, 454.

J.L.Tallon. (1980). *J. Phys. Chem. Solids,* 41, 837.

K.S.Singh, R.S.Chauhan. (2002). *Physica,* B 315, 74.

K.Y.Singh, B.R.K.Gupta. (2003). Physica B 334, 266.

O.L.Anderson, D.Issak, H.Oda, (1992). *Rev.Geophys*., 30, 57.

O.L.Anderson. (1995). Equation of State for Geophysics and Ceramic Sciences, Oxford University Press, Oxford.

R.S.Chauhan, C.P.Singh. (2007). *Physica* B 387, 352.

S.K.Srivastava, Physica. (2005). B 363, 122.

X.Q.Deng, Z.T.Yan. (2002). *J. Phys. Chem. Solids*, 63, 1737.

Z.H.Fang. (2005). *Physica B* 357 433.

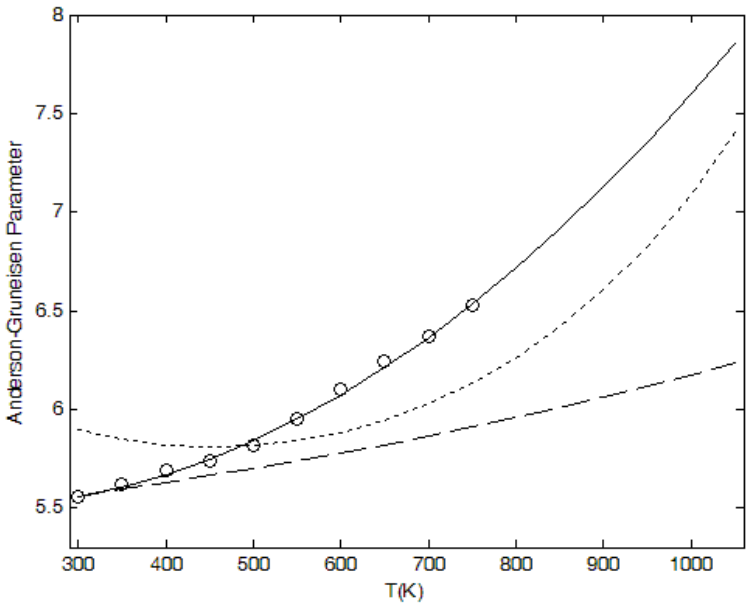

Figure 1. Predicted values of Anderson–Gruneisen parameter at different temperatures for NaCl. Dotted line - Eq.(4), dashed line — Eq. (7), solid line — the present model Eq.(8), empty circle — experimental data from [O.L.Anderson, 1992]

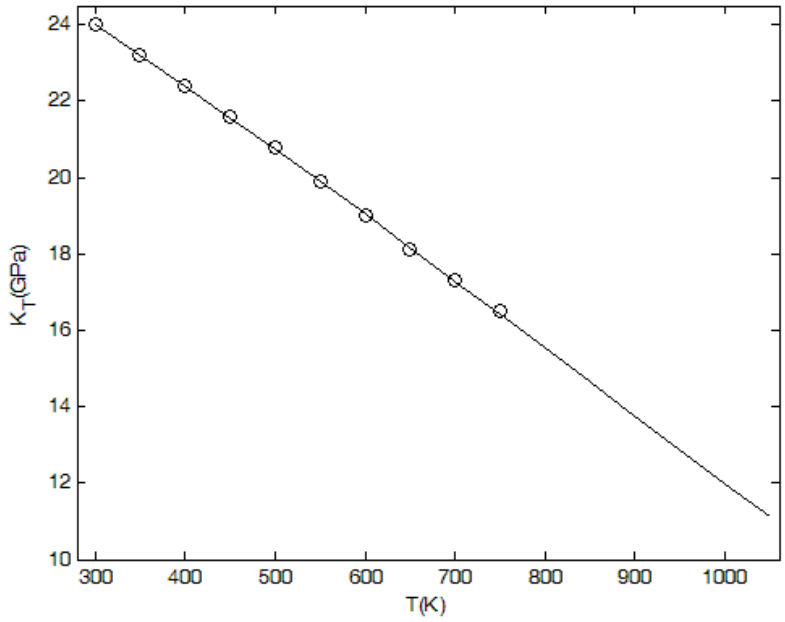

Figure 2. Predicted values of the isothermal bulk modulus at different temperatures for NaCl. solid line — the present model Eq.(9), empty circle — experimental data from [O.L.Anderson, 1992].