Review of: "High-pressure thermal conductivity and compressional velocity of NaCl in B1 and B2 phase"

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The present work brings light on the pressure-induced structural phase transition from phase B1 to B2 in sodium chloride (NaCl) at room-temperature. The author presents very interesting experimental results, which are discussed in terms of the connection between the thermal conductivity and the effective Grüneisen parameter γ via the so-called Leibfried-Schlömann (LS) equation. It is known that the above-mentioned structural phase transition is accompanied by an entropy change of (1.5 ± 0.3) cal·deg^{-1} under a pressure of 300 kbar and a volume change of (-1.00 ± 0.05) cm^{3}·mole^{-1}, cf. Ref. [1]. It has been discussed in the literature that γ and the so-called Grüneisen ratio (GR) are powerful tools to explore both phase transitions and critical phenomena, following discussions presented in Refs [2-8] and references cited therein. This is because γ, as well as the GR, quantifies the entropy change associated with the phase transition of interest upon varying both temperature and the control parameter. In the present case, the author considers γ as a constant at phases B1 and B2 in the analysis of the results.

It is of interest to analyze the behavior of γ and GR close to the B1-to-B2 structural phase transition. It is unclear whether such a structural transition is mean-field-type or not. It is well-known that the Ginzburg criterion dictates the region in which fluctuations starts to play a key role [9]. Hence, in the present case, it would be of interest to explore the character of the phase transition, as well as to establish its corresponding Ginzburg criterion. The volume dependence of γ was discussed into details in Ref. [1], namely:

$$(\partial ln\gamma/\partial lnV)_T = 1 - \alpha^{-1}(\partial lnB_T/\partial T)_V - (\partial lnC_V/\partial lnV)_T,$$

where B_T, C_Vrefer, respectively, to the bulk modulus and the specific heat at constant volume. It turns out that the entropy of the system is changed under 300 kbar as a consequence of the volume change associated with the structural phase transition, cf. Fig. 2 of Ref. [1]. Hence, it is natural to expect that γ varies in the vicinity or at the transition. In other words, γ does not vary too much far from the phase transition, cf. literature results [6]. However, at or close to the B1-to-B2 structural phase transition under 300 kbar, it is expected that γ is no longer constant.

Thus, it would be desirable to explore the behavior of γ closer to the B1-to-B2 structural phase transition in

sodium chloride, which is depicted as the highlighted region in pink color in Figs. 1, 3, 4, and 5 of the present work.

Congratulations to the author for the nice work!

References

[1] W.A. Bassett, T. Takahashi, H. Mao, J.S. Weaver, J. Appl. Phys. **39**, 319 (1968). DOI: https://doi.org/10.1063/1.1655752

[2] M. de Souza, P. Menegasso, R. Paupitz, A. Seridonio, R.E. Lagos, Eur. J. Phys. **37** 055105 (2016). DOI: https://doi.org/10.1088/0143-0807/37/5/055105

[3] L. Bartosch, M. de Souza, M. Lang, Phys. Rev. Lett. **104**, 245701 (2010). DOI: https://doi.org/10.1103/PhysRevLett.104.245701

[4] G.O. Gomes, L. Squillante, A.C. Seridonio, A. Ney, R.E. Lagos, M. de Souza, Phys. Rev. B **100**, 054446 (2019). DOI: https://doi.org/10.1103/PhysRevB.100.054446

[5] L. Squillante, I.F. Mello, G.O. Gomes, A.C. Seridonio, R.E. Lagos-Monaco, H.E. Stanley, M. de Souza, Sci. Rep. **10**, 7981 (2020). DOI: https://doi.org/10.1038/s41598-020-64632-x

[6] I.F. Mello, L. Squillante, G.O. Gomes, A.C. Seridonio, M. de Souza, J. Appl. Phys. **128**, 225102 (2020). DOI: https://doi.org/10.1063/5.0018604

[7] L. Squillante, I.F. Mello, A.C. Seridonio, M. de Souza, Sci. Rep. **11**, 9431 (2021). DOI: https://doi.org/10.1038/s41598-021-88778-4

[8] L. Squillante, I.F. Mello, A.C. Seridonio, M. de Souza, Mat. Res. Bull. **142**, 111413 (2021). DOI: https://doi.org/10.1016/j.materresbull.2021.111413

[9] J. Als-Nielsen, R.J. Birgenau, Am. J. Phys. 45, 554 (1977). DOI: http://dx.doi.org/10.1119/1.11019