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Reply to Comment

Reply to : "Comment on the paper 'Analysis of thermal expansivity of alkali halide crystals' : NaF as an example"

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In the present Comment, Kumar *et al* have made a case against the recent work on thermal expansivity of alkali halides published by Singh and Chauhan [1]. However, the Comment by Kumar *et al* is a very weak one and the arguments given are not valid for the reasons given below :

(1) This is true that there are few misprints in the paper by Singh and Chauhan [1], for example the fourth column D for NaF in Table 3 and caption to Figures 2–4. In fact, the original version of the paper contained the plots for all the eight crystals, but following a suggestion made by the referee, they were reduced to three only. However, the correction could not be made in the caption to Figures 2–4. This is an easily understandable happening but Kumar *et al* have written unwanted statements (one can see the last paragraph written by them on pages 5 and 6, and the similar statements also given in the beginning).

(2) The mistake in printing of one column only for NaF encouraged Kumar *et al* to write a paper. Why did they not include remaining seven crystals in their analysis? Certainly, NaF cannot be an example, which they have mentioned in the title of the paper.

(3) Singh and Chauhan [1] have rectified an error in the formula of thermal expansivity α adopted by Kumar [3].

$$\alpha = \alpha_0 + \alpha' T. \quad (1)$$

Eq. (1) was not consistent as it does not yield $\alpha = \alpha_0$ at $T = T_0$. So eq. (1) was modified as

$$\alpha = \alpha_0 + \alpha'(T - T_0). \quad (2)$$

It was found by Singh and Chauhan [1] that this correction modified significantly the final results for the temperature dependence of interatomic distances in case of alkali halides.

(4) In the present Comment, Kumar *et al* emphasised that their eq. (1) is correct. They redefined the boundary condition $\alpha = \alpha_0$ at $T = 0$. However, Singh and Chauhan performed their analysis by revising the Kumar analysis given in Ref. [3]. In that paper, Kumar has taken $\alpha = \alpha_0$ at $T = T_0$ and not at $T = 0$. One can easily verify from Ref. [3] that the values of α_0 are at 300 K which is also the initial temperature taken by Kumar in his calculations. Singh and Chauhan have emphasised that eq. (1) is not valid when α_0 represents the thermal expansivity at $T_0 > 0$.

(5) Kumar *et al* have used eq. (7) to justify the validity of eq. (4). It should be mentioned that at $T = 0$, eq. (7) yields $\alpha_0 = 3.912 \times 10^{-5}$ which is not the value for NaCl at room temperature. Thus, α_0 in eq. (8) is not the value of α at $T = T_0$. On the other hand, in eq. (4) of Kumar *et al*, α_0 is certainly the value of α at $T = T_0 = 300$ K [3]. Thus, eq. (4) is not

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consistent with the boundary condition at $T = T_0$ for which α_0 corresponds. This has clearly been demostrated in the paper by Singh and Chauhan (First paragraph of 'Results and Discussions' and the results given in Table 2).

(6) As mentioned in our paper [1] we have taken guidance from Dr. Jai Shanker. It is worth mentioning here that Dr. M Kumar also completed his PhD under the guidance of Dr. Jai Shanker.

Reference

[1] C P Singh and R S Chauhan *Indian J. Phys.* **78** 1215 (2004)