Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

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Thermal expansion of the alkali halides.

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From comparison of results of measurements of the coefficients of thermal expansion of the alkali halides using X-ray diffraction methods and dilatometer and interferometer methods, it is claimed that the non-linearity of the thermal expansion is due to anharmonic effects and not to defect formation.

The form of the variation of the coefficient of thermal expansion with temperature has been found to be similar for all the alkali halides. From room temperature, the coefficient increases linearly with temperature up to approximately 200°K degrees below the melting point where a so-called 'anomalous' increase in the coefficient takes place. This 'anomalous' increase has been attributed by many authors, *e.g.* Enck & Dommel (1965), to the formation of thermally generated Schottky defects. Leadbetter & Newsham (1969), however, have suggested that this behaviour is more likely due to an anharmonic effect.

Two recent papers, Pathak & Vasavada (1970), Paper I, and Pathak, Trivedi & Vasavada (1973), Paper II, report the measurements of the coefficient of thermal expansion in the range of temperature from room temperature to the melting point for six alkali halides and the results confirm the so-called 'anomalous' temperature dependence of the coefficient. The authors attribute the variation of the expansion coefficient from linearity to defects and calculate, by a method suggested by Enck & Dommel (1965), the energies of formation of these defects. The measurements quoted in these papers were made by the X-ray diffraction method which utilizes Bragg's Law in determining the size of the unit cell in the crystal. The formation of Schottky defects will not alter the size of the unit cell in the crystal and while the production of a very large number of Frenkel defects may cause an enlargement of very many unit cells, it is extremely unlikely that sufficient of these defects could be introduced into an alkali halide to produce any movement in the Bragg peak. Defects, therefore, cannot have any effect on the coefficient of thermal expansion measured by the X-ray diffraction method. It must be concluded that the non-linearity of the thermal expansion coefficient of the alkali halides is not due to defect formation and that the deductions made in Papers I and II are incorrect.

If bulk-sample enlargement due to defect formation is taking place, expansion coefficients measured using the X-ray diffraction technique should be less than those measured using either dilatometer or interferometer methods. Results from X-ray measurements for sodium chloride are given in Paper I with dilatometer results (Leadbetter & Newsham, 1969) and interferometer results (Enck & Dommel, 1965) and it can be seen that all results show the same non-linearity at high temperatures. The X-ray diffraction method results are slightly higher than the results from the dilatometer experiment at high temperatures but slightly lower than those from the interferometer experiment. The values quoted in Paper I for potassium chloride show the X-ray diffraction method gives significantly higher coefficients of expansion than the interferometric method (Enck, Engle & Marks, 1962) but very similar results to the dilatometer method (Leadbetter & Newsham, 1969). These results suggest that if defects play any part in the thermal expansion of the alkali halides, their role must be a minor one and the 'anomalous' behaviour of the coefficient of thermal expansion is likely to be due to third and higher-order terms in the potential energy.

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