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Some aspects of the phase transformation in solid CsCl

Weijma, Hette

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SUMMARY

Of the twenty alkali halides seventeen crystallize in the NaCl or B1-structure at room temperature and atmospheric pressure. Only CsCl, CsBr and CsI possess the CsCl or B2-structure under S.T.P. conditions. CsCl, however, transforms from the B2 into the B1 structure at a temperature of 476°C under atmospheric pressures. The reverse B1→B2 transition takes place at 471°C.

This thesis deals with some of the physical aspects of the B2⇌B1 phase transformation in CsCl. In particular, the kinetics of the transition have been studied in order to obtain an insight into the mechanisms of the transformation. The ionic conduction mechanism in CsCl and the influence of Ba²⁺, Rb⁺, K⁺ and Br⁻-ions on the phase transition have also been investigated.

Chapter 1 is devoted to the polymorphism occurring in several alkali halides. A short survey is given of the available literature data about the phase transition in CsCl.

The experimental procedures are described in Chapter 2. Single crystals have been grown by means of the Kyropoulos-Czochralski method. Measuring techniques include experiments on the electrical conductivity and the linear expansion, both as a function of temperature, and a differential thermal analysis (D.T.A.).

The conductivity of CsCl has been measured for sample temperatures ranging from about 260 to about 620°C (Chapter 3). Employment of Ba²⁺-doped crystals has provided a powerful tool for the study of the conduction mechanisms. In both the B2 and the B1 structure the activation enthalpies and ionic mobilities have been determined. The results have been explained in terms of the cation and anion vacancy migration. The contribution of the anion vacancies in B2-CsCl has been established to be over 80% of the total conductivity.

Chapter 4 deals with the phase transformation phenomena in CsCl-RbCl, CsCl-KCl and CsCl-CsBr mixed crystals. As might be expected from the thermodynamical properties of RbCl and KCl the addition of a few molar percents of one of these chlorides to CsCl reduces considerably both the transition temperature and the latent heat relative to those of pure CsCl. On the other hand, addition of CsBr to CsCl raises the transition temperature but lowers the latent heat. It is concluded that pure CsBr would exhibit a B2→B1 transformation at 805°C, i.e. far above its melting point of 636°C, involving a latent heat of about 380 cal/mole (CsCl:707 cal/mole).

In Chapter 5 and 6 we report on the kinetics of the $B2 \rightleftharpoons B1$ transition in CsCl. The necessary framework of equations is developed in Chapter 5. The progress of the transformation is studied by means of conductivity and linear expansion measurements, carried out both while the crystal is heated at a uniform rate and cooled in the same way (Chapter 6). The results indicate that the transition is diffusion controlled, i.e. nucleation and growth processes dominate. The Avrami and Johnson-Mehl formalisms have been used for the evaluation of the kinetics of the transformation. During the first stage of the $B2 \rightarrow B1$ transition, in which about 98% of the material transforms, the new phase grows uniformly in the form of ellipsoidal particles, while the nucleation rate is constant. The final stage may be considered as a first order rate process. The rate constant occurring in the Avrami formalism depends on the heating and cooling conditions as well as on the thermal history of the crystal.