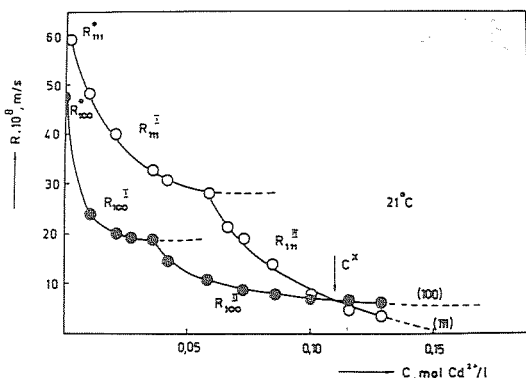


07.1-13 INFLUENCE OF CADMIUM IONS ON THE LINEAR CRYSTAL GROWTH RATE OF POTASSIUM HALIDES: THE SYSTEM $\text{KBr}-\text{CdBr}_2-\text{H}_2\text{O}$. By D. Draganova, R. Koleva, Faculty of Chemistry, Sofia University, 1126 Sofia, Bulgaria.

This reports the effect of cadmium ions on the growth of potassium bromide crystals on the basis of the $R_{100}(C)$ and $R_{111}(C)$ curves, where R is the growth rate and C is the impurity concentration. The R -values were measured under stationary conditions by Bliznakov's method. The experimental data at 21°C , shown on fig. 1, as well as the data at 25 and 30°C , lead to the conclusion that cadmium ions are adsorbed and incorporated in KBr crystals according to two different mechanisms: I and II.



The mechanism I probably occurs through the adsorption of the complexes CdBr_2^{2-n} ($n < 6$), which turn into CdBr_6^{4-} in the adlayer and enter the crystal lattice. Estimated from the $R(C,T)$ curves the adsorption heats Q ($\text{kcal}\cdot\text{mol}^{-1}$) are quite high: $Q_{100}^I \times Q_{111}^I = 14$. It seems that these Q -values include additional heat for the complex formation on the crystal surface.

The $R(C)-I$ curves follow the equation of Bliznakov (Fortschr. Min. (1958) 36, 149), which permits the calculation of the surface diffusion activation energy for the adsorbed impurity complexes: 1075 cal for (100) and 720 cal for (111) KBr .

The mechanism II is a result of the formation of two-dimensional adsorption phases. That is why $Q_{111}^{II} > Q_{100}^{II}$ ($Q_{111}^{II} = 8.2$; $Q_{100}^{II} = 5.1$) and this leads to the habit transition (100) \rightarrow (111) in the C -range of II, according to the relation given by Draganova:

$$\lg C^X = \text{const} + \frac{Q_{100}^{II} + Q_{111}^{II}}{2 \times 2.3 RT}$$

Here C^X is the C -value, for which $R_{100} = R_{111}$ at the corresponding T .

These data seem to give a good explanation of two well known crystallographic phenomena: a) minute impurity traces stimulate the growth of more perfect single crystals - mechanism I with strong passivating effect, but without any change in the R_{100}/R_{111} ratio; b) habit modifications always occur at higher C -values. The succession of the action of mechanisms I and II and their different temperature dependence is the reason for the low concentration limits of the impurity habit changing activity.

07.2-01 MULTI-CELL-SIZE LATTICE MODELS APPLIED TO THE INTERPRETATION OF SMALL-ANGLE X-RAY SCATTERING DATA FOR CATALYSTS. By J. Goodisman and H. Brumberger, Dept. of Chemistry, Syracuse University, Syracuse, NY 13210.

Multi-cell-size models, employing spherical or cubic cells with different size distributions to represent the solid catalyst phase are used to interpret the observed small-angle X-ray scattering of two-phase (void-solid) Al_2O_3 catalysts. Theoretical scattering intensities are calculated from the correlation functions for these models, and the intensities are then numerically smeared for comparison with experimental data taken under "infinite slit" conditions. These models predict the bimodal form of the first moment of the slit-smeared intensity which appears to be appropriate for a number of catalysts.

07.2-02 THE STRUCTURES OF EQUILIBRIUM AND MELTING LENNARD-JONES CRYSTAL-MELT INTERFACES. By G. Bushnell-Wye and J. L. Finney, Crystallography Dept, Birkbeck College, Malet Street, London, WC1E 7HX, England, and A. Bonissent, Centre de Recherche sur les Mécanismes de la Croissance Cristalline, Campus de Luminy, Case 913, 13288 Marseille Cedex 2, France.

Monte Carlo calculations have been performed on the Lennard-Jones crystal-melt interface (the 0001 face of the h.c.p. system), both (a) slightly above and (b) at the triple point, to investigate the nature of the interface at equilibrium and on melting. The boundaries of the very large systems simulated (about 4500 atoms) were periodic along the interface. Ten layers of crystal were allowed to move under the Monte Carlo process, and these were bounded below by four further layers which remained fixed. The liquid region extended to about 20 layers above the interface, and its surface was either confined (to simulate constant volume) or free.

A hard sphere model of the interface was used as the starting configuration (Bonissent and Mutaftschiev, Phil. Mag. B35, 65, 1977). About 5×10^6 configurations have been calculated for the elevated temperature assembly, which begins to show the onset of melting. Unlike the behaviour observed in smaller assembly calculations (Bonissent, Gauthier and Finney, Phil. Mag. B39, 49, 1979), atoms moved in from both the liquid and crystal sides of the interface removing the density deficit observed at the interface in the earlier hard sphere models. Thus, in contrast to homogeneous simple liquids where the essential physics can be argued to be contained in the hard sphere structure, the severity of the packing constraints at a hard sphere interface seems to give rise to behaviour which is qualitatively different from the more realistic soft sphere case modelled here. Atom movements into the interfacial region from the crystal, together with plots of density profiles across the