07.1-13   INFLUENCE OF CADMIUM IONS ON THE LINEAR
CRYSTAL GROWTH RATE OF POTASSIUM HALIDES: THE SYSTEM
KBr-CdBr$_2$-H$_2$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 stationery 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.
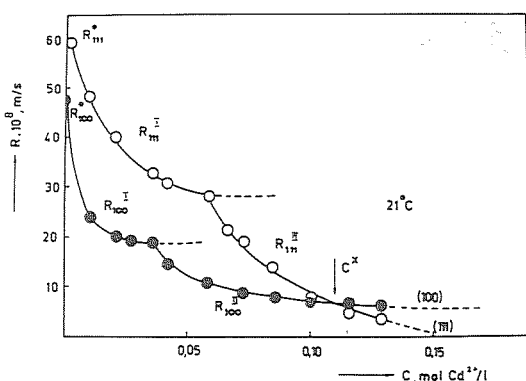
The mechanism I probably occurs through the adsorption of
the complexes CdBr$_n^{2-n}$ (n<6), which turn into CdBr$_6^{4-}$ in
the adlayer and enter the crystal lattice. Estimated
from the R(C,T) curves the adsorption heats Q (kcal.mol^{-1})
are quite high: Q_{100}xQ_{111}=14. It seems that these Q-
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 cal-
culation 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)→(111) in the C-range of II,
according to the relation given by Draganova:

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

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,
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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$_2$O$_3$ catalysts. Theoretical scattering
intensities are calculated from the correlation
functions for these models, and the intensities are
then numerically smeared for comparison with experi-
mental 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 inter-
face 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 X 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 ob-
served 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