

15-Crystal Growth

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PS-15.02.22 SURFACE SUPERSATURATION ON GROWING OF CRYSTAL

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Supersaturation σ_s on growing surface of crystal as a function of volume supersaturation σ is nonlinear and determined by equation (Askhabov, 1993):

$$\sigma_s = \frac{\sigma^*}{2} \left[\left(1 + \frac{4\sigma}{\sigma^*} \right)^{1/2} - 1 \right]$$

The parameter σ^* in (1) depends mainly on correlation of volume diffusion and surface kinetics processes during crystal growth. The values of σ^* for the growing faces of crystal are found based on experimental data $R(\sigma)$, where R is growth rate of crystal faces. Equation (1) may be used for determination $\sigma_s(\sigma)$ for the crystal growing in the conditions of free and forced convection. For example, for the K-alum crystals growing in the free convection condition, the dependences $\sigma_s(\sigma)$, based on experimental data $R(\sigma)$ are following:

$$\sigma_s = 0.02[(1 + 100\sigma)^{1/2} - 1] \text{ for } \{111\}$$

$$\sigma_s = 0.031[(1 + 64.5\sigma)^{1/2} - 1] \text{ for } \{001\}$$

On the growth center σ_s is more, then one far from center. Because of it, gradients of supersaturation are appear on the face, and cause the formation of macrosteps. When the gradient achieve critical values the morphological stability of growing crystal faces are lost. For the crystal growing in the dynamic conditions, σ_s achieves 0.80-0.90. Absolutely kinetic regime for the crystal growth from solution can not be achieved. That's why only experimental dependences $V(\sigma_s)$, got as result of calculations σ_s from σ , can be compared to theoretical models of crystal growth.

References: A. M. Askhabov, Crystal growth from solution. Syktyvkar, 1993, 22p (Russ.)

PS-15.02.23 GROWTH DEFECT INVESTIGATIONS IN SILVER THIOGALLATE.

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Silver thiogallate, AgGaS_2 , is a well known commercial crystal for nonlinear application and belongs to the chalcopyrite type structure. As a rule, AgGaS_2 crystals exhibit twinning defects in $\{112\}$ crystallographic planes and there is a problem in obtaining crystals of sufficient size which contain no defects and could be used in optical elements manufacture. The crystals of different technological stages of synthesis and growth have been investigated by Infra-red and Raman spectroscopy methods. The nonstoichiometry can result in appearance of modes forbidden by ideal symmetry in the region of atoms valence vibration. Thus IR spectra of some powder samples have an absorption band at 300 cm^{-1} assigned to A_1 forbidden mode. A single crystal used in the Raman measurements has been grown by Bridgeman-Stoobarger technique and orientated along the principal crystallographic axes.

At examination in polarized microscope the sample looks like one large domain with visible twinning defects in $\{112\}$ plane at one

end. From the low-energy side of the A_1 (295 cm^{-1}) mode one can observe a 275 cm^{-1} mode as a shoulder which was identified as vacancy-sulphur vibration rather than the second-order, the structure of which vanishes at 80K. As a result of our experimental study of the defects present in AgGaS_2 it is possible to discuss the influence of stoichiometry on the optical quality of single crystals and twinning phenomena.

PS-15.02.24 ON THE PREPARATION OF $11\text{CaO} \cdot 7\text{Al}_2\text{O}_3 \cdot \text{CaF}_2$ SINGLE CRYSTAL.

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The preparation of $11\text{CaO} \cdot 7\text{Al}_2\text{O}_3 \cdot \text{CaF}_2$ ($\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$) for short in the following) single crystals is important for the analysis of its structure. Generally it is recognized that it is impossible to obtain a stoichiometric $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ crystal due to the evaporation of fluorine at high temperature. After studying the growing mechanism, dynamics and proper conditions $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ single crystals with a trigonal tritetrahedron habit of $40 \sim 120 \mu\text{m}$ have been prepared for the first time by using appropriate amount of PbCl_2 as flux. The formation process and stability of $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ at high temperatures as well as the effect of doped ions on them have also been determined by Powder XRD, QXRD, IR spectrum, Raman spectrum, HT—DTA and HTM techniques with the theory and methods of solid chemistry and physical chemistry. The results show that the formation mechanism of $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ at high temperature is in accordance with the equation suggested by Ginstling—Brounshetein, and if there is an appropriate amount of fluorine in the raw meal the final product is only $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ and no other calcium aluminates such as C_{12}A_7 and C_3A can be found. Based on sufficient experimental results and theoretical deduction we have concluded that $\text{C}_{11}\text{A}_7 \cdot \text{CaF}_2$ is congruently melted at 1465°C .