

08.4-21 THE MODULATED STRUCTURE OF THE e-PLAGIOCLASE FELDSPARS. By M. Kitamura and N. Morimoto, Department of Geology and Mineralogy, Kyoto University, Kyoto, 606, Japan and A. Yamamoto and H. Nakazawa, National Institute for Research in Inorganic Materials, Sakura-Mura, Niihari-Gun, Ibaraki 305 Japan.

The modulated structure of labradorite (An_{52}) has been refined within the harmonic approximation using the intensity data collected by Klein (Horst et al., Z.Krist. (1981) 157, 233) resulting in the R factor of 0.078 in which $R_0=0.066$ for 1640 main (a) and $R_1=0.105$ for 3220 e_1 -satellite reflections by the present authors (Yamamoto et al., Acta Cryst. (1984) B40 in press). These values can be compared with the previous factors obtained by Horst et al. (1981) using the same intensity data: $R=0.080$, $R_0=0.066$ and $R_1=0.182$.

This structure determination indicates that the most probable structure of labradorite is a modulated one in which the anorthite-like (An_{80}) regions in an antiphase relation are coherently separated by the albite-like (An_{20}) regions, being consistent with the KM-structure model presented by Kitamura and Morimoto (Phys. Chem. Miner. (1977) 1, 199). Comparison of this KM-model with other previously presented models indicates that only the KM-model can explain the continuous change of the modulated structure by composition in the e-plagioclase series (An_{25} - An_{75}). The KM-model also supports resonance structures between the Ca-rich I-anorthite and Na-rich I-albite which stabilize the e-plagioclase series.

08.4-22 A GEOMETRICAL INTERPRETATION OF THE STRUCTURAL PARAMETER OF CHALCOPYRITE ($E1_1$) TYPE COMPOUNDS ABC_2 . By P. Paufler and P. ROITSCH, WB Kristallographie, Sektion Chemie, Karl-Marx-Universität, Leipzig, DDR.

Distances d between different A, B, and C atoms up to $d \approx \alpha$ have been investigated as a function of the structural parameter, u , and the axial ratios $c/a = \alpha$ (c, α lattice parameters). Those parameters $u = u_0$ for which certain distances are equal fulfil relations $u_0 = f(\alpha)$ that were evaluated. They have been compared to experimental data $u_{exp} = f(\alpha_{exp})$. It is shown that the structural parameters observed may be interpreted by the equality of certain atomic distances $d \approx (0.7 \dots 0.8)\alpha$ beyond next neighbour distances $d \approx (0.4 \dots 0.5)\alpha$. Different bonds are dominating in different representatives of that structure. The regular tetrahedra condition as proposed by Abrahams and Bernstein (J.Chem.Phys. 55, 796 (1971)) turns out as a special case which applies only for part of the compounds.

08.4-23 ORIENTED INTERGROWTH OF CORUNDUM IN DIAMOND CRYSTALS. By W.G.R. de Camargo, Institute Geosciences, University of São Paulo, Brazil & L.A.R. de Camargo, Escola de Engenharia Mauá, S. Paulo, Brazil.

Several oriented intergrowths have already been described between diamond hosts and their solid inclusions. In addition, some other possible intergrowths have been suggested in diamond crystals, such as enstatite, diopside, spinel, rutile, ilmenite, etc., by considering the lattice similarities of the host and their inclusions.

Meyer and Gubelin (Ruby in diamond, Gems and Gemology, 1981, pg. 153) described for the first time, red corundum inclusions (ruby) in diamond crystals of unknown origin. These authors had no evidences for an epitaxial relationship, but suggested a possible crystallographic orientation of the two minerals at conditions of higher temperatures and pressures, in which both crystals were formed.

By taking into account the lattice constants of diamond and corundum, there is a fairly good possibility of an epitaxial growth of corundum crystals ($a_0 = 4.76$ Å, $c_0 = 12.99$ Å) on the (111) faces of diamond ($a_0 = 3.56$ Å). By a further growth of the host crystal the corundum remained as an inclusion in the diamond.

Corundum crystals may be developed on the (111) diamond faces, which correspond to the densest lattice plane of diamond, according to the following intergrowth relationships:

	Diamond	Corundum
Intergrowth common face	(111)	(0001)
Lattice row 1	$[\bar{1}\bar{1}0]$	$[\bar{1}2\bar{1}0]$
Lattice row 2	$[10\bar{1}]$	$[2\bar{1}\bar{1}0]$
Angle 1/2	60°	60°
Identity periods	5.035 Å = $2T[\bar{1}10]$	4.76 Å = $1T[1120]$
Misfit in both rows	0.275 Å $\sim 5.8\%$	

b) for prismatic corundum crystals

	Diamond	Corundum
Intergrowth common face	(111)	(10 $\bar{1}$ 0)
Lattice row 1	$[\bar{1}\bar{1}0]$	$[\bar{1}2\bar{1}0]$
Identity period	5.035 Å = $2T[\bar{1}10]$	4.76 Å = $1T[1120]$
Misfit	0.275 Å $\sim 5.8\%$	
Lattice row 2	$[11\bar{2}]$	$[0001]$
Identity period	13.02 Å = $3T[112]$	12.99 Å = $1T[0001]$
Misfit	0.03 Å $\sim 0.3\%$	
Angle 1/2	90°	90°

The elongated corundum (ruby) inclusions, parallel to the c - crystallographic axis, as described by Meyer & Gubelin (1981), possibly suggest the b) case of oriented intergrowth.