M. Korekawa, W. Horst, and T. Tagai (Inst. f. Krist. und Min. der Univ. Frankfurt/M). **Determination of Superstructure of Labradorite $An_{\sim 50}$.**

The superstructure of labradorite, An_{54} (Labrador), was determined according to an extended theory of satellites. The extended theory explains the fact that almost all the observed satellites are the first order satellites (e-reflections), and that the higher order satellites expected in the area of higher glancing angles in case of shift modulation model do not appear (Jagodzinski and Korekawa, 1978; Korekawa et al., 1978). The superstructure is described as the periodic antiphase domains with the boundaries (APB) nearly parallel to $(11\bar{4})$, which refers to $c \sim 14$ Å. It consists of two centrosymmetric structure elements ϱ_1 and ϱ_2 (Fig. 1 b), which are arranged in the way shown in Figure 1 a.

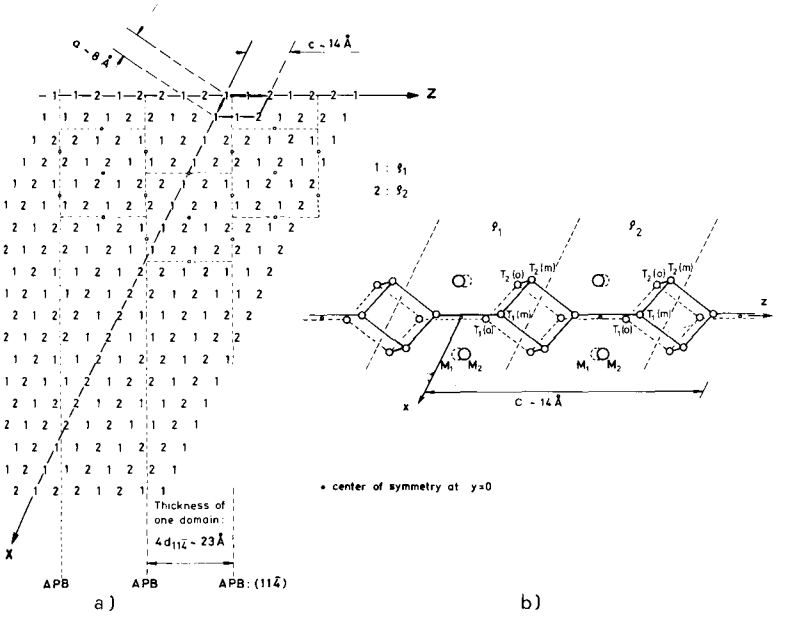

Fig. 1. a Section of idealized superstructure of $An_{\sim 50}$ (schematic). **b** A part of the averaged "body-centered structure" (schematic)

At the first stage of structure determination two hypothetical "body-centered structures" ($c \sim 14$ Å with $I\bar{1}$) were introduced using the e-reflections with $(+\delta h, +\delta k, -\delta l)$ and those with $(-\delta h, -\delta k, +\delta l)$, respectively, indexed as the corresponding b-reflections, namely neglecting δh, δk, and δl. These "body-centered structures", in each of which specific ϱ_1 is at 0,0,0 and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$, and specific ϱ_2 at $0,0,\frac{1}{2}$ and $\frac{1}{2},\frac{1}{2},0$, respectively, were refined independently and then averaged. The averaged body-centered structure was deconvoluted into the superstructure according to the scheme given in Fig. 1a and refined with center of symmetry by the least squares program ORXFLS, which is modified for this problem. The overall R-factor is attained to 4.7% for 877 a-reflections and 1663 e-reflections, including zero intensities ($R_{a\text{-ref.}} = 2.8\%$ and $R_{e\text{-ref.}} = 21\%$; Cu-K_α with absorption correction). The averaged T−O bond lengths and atom coordinates for the structure elements ϱ_1 and ϱ_2 are given in the following tables (preliminary values).

In the course of superstructure refinement some atoms apparently show relatively large anisotropic temperature factors, which may be mainly caused by the positional disorder in each structure elements (cf. ⟨T−O⟩ values in Table 1). The periodicity of the superstructure is interpreted by the modu-

Table 1. Averaged T–O bond lengths: ⟨T–O⟩

Atom	ϱ_1 ⟨T–O⟩ [Å]	ϱ_2 ⟨T–O⟩ [Å]
T_1 (o)	1.670	1.705
T_2 (o)	1.660	1.629
T_1 (m)	1.670	1.628
T_2 (m)	1.634	1.669

Table 2. Atom coordinates (referred to c ~ 7 Å)

Atom	ϱ_1			ϱ_2		
	x	y	z	x	y	z
M_1	0.2722(4)	0.0269(4)	0.1015(4)	0.2700(3)	0.0303(2)	0.1007(2)
M_2	0.2692(3)	0.9825(4)	0.1663(3)	0.2665(6)	0.9705(8)	0.1714(5)
T_1 (o)	0.0069(2)	0.1639(1)	0.2116(1)	0.0055(2)	0.1658(1)	0.2171(1)
T_2 (o)	0.6876(2)	0.1106(1)	0.3161(1)	0.6845(2)	0.1081(1)	0.3180(1)
T_1 (m)	0.0021(2)	0.8165(1)	0.2335(1)	0.0048(2)	0.8184(1)	0.2294(1)
T_2 (m)	0.6809(2)	0.8808(1)	0.3595(1)	0.6832(2)	0.8781(1)	0.3549(1)
O_A (1)	0.0062(5)	0.1299(3)	0.9800(2)	0.9973(6)	0.1293(4)	0.9768(3)
O_A (2)	0.5834(5)	0.9932(3)	0.2797(3)	0.5812(4)	0.9925(2)	0.2784(2)
O_B (o)	0.8141(5)	0.1060(3)	0.1873(3)	0.8099(5)	0.1055(3)	0.1928(3)
O_B (m)	0.8147(5)	0.8532(3)	0.2512(3)	0.8193(5)	0.8534(3)	0.2405(3)
O_C (o)	0.0139(4)	0.2906(3)	0.2774(3)	0.0154(4)	0.2941(3)	0.2818(3)
O_C (m)	0.0161(4)	0.6863(3)	0.2194(2)	0.0165(5)	0.6916(6)	0.2128(4)
O_D (o)	0.1947(5)	0.1085(3)	0.3833(2)	0.2011(5)	0.1074(3)	0.3848(2)
O_D (m)	0.1925(4)	0.8671(3)	0.4328(3)	0.1859(5)	0.8665(3)	0.4304(3)
	M_1: $Ca_{17}Na_{33}$; M_2: $Ca_{25}Na_{25}$			M_1: $Ca_{39}Na_{11}$; M_2: $Ca_{29}Na_{21}$		

lation of the structure elements ϱ_1 and ϱ_2, which contains the density modulation (Ca/Na) with the same wavelength. The disorder at domain boundaries (APB) and fluctuation of periodicity will be discussed.

Literature

H. Jagodzinski, M. Korekawa: Phys. Chem. Minerals **3** (1978) 69–72
M. Korekawa, W. Horst, T. Tagai: Phys. Chem. Minerals **3** (1978) 74–75