A CRYSTAL STRUCTURE REFINEMENT OF AN ANOMALOUS LUNAR ANORTHITE; Joseph R. Smyth, The Lunar Science Institute, 3303 NASA Rd. 1, Houston, TX 77058.

Lunar sample 76535 is a coarse-grained troctolytic granulite composed of plagioclase (58 percent, An\textsubscript{95}), olivine (37 percent, Fo\textsubscript{88}), and orthopyroxene (4 percent, En\textsubscript{86}). The rock has been described in detail by Gooley \textit{et al.} (1) who have inferred that it represents a cumulate which was deposited at a depth of 10 to 30 km in the moon, and that subsequent cooling rates were on the order of a few tens of degrees per million years. The individual major mineral grains are large (up to 3 mm in greatest dimension), homogeneous, and show no evidence of shock. If the conclusions of Gooley \textit{et al.} (1) are correct, this sample is one of the most slowly cooled and well-equilibrated bits of silicate material yet described and offers a unique opportunity to study crystal-chemical ordering processes in the three major minerals.

Several authors (2,3,4) have noted that lunar plagioclase feldspars in general, show larger deviations from the ideal formula,

$$\text{Na}_x \text{Ca}_{1-x} \text{Al}_{2-x} \text{Si}_{2+x} \text{O}_8$$

than do terrestrial feldspars. The deviations are discussed in detail by Wenk and Wilde (3) who state that most lunar plagioclases tend to be Na-poor or Si-rich and propose several substitutions to account for the observed anomalies. The chemical analysis for 76535 plagioclase (in numbers of atoms per eight oxygens) is: Si, 2.077; Al, 1.927; Fe, 0.002; Ca, 0.932; Na, 0.145; and K, 0.022. The chemical anomaly in this plagioclase is clearly shown by comparing the An-content calculated from the Al-Si ratio (92.4) to that of the Ca/(Ca+Na+K) ratio (95.7) despite the near absence of Fe and Mg.

Long-exposure (168-hour) precession photographs of the feldspar show diffractions consistent with space groups \textit{P}_{\text{1}}\text{I} and \textit{P}_{\text{1}}. All classes of reflection (a, b, c, and d) are present and of equal sharpness as is consistent with extremely slow cooling for this composition (5). Cell dimensions:

- \(a = 0.8173\) (2) nm  \(\gamma = 93^{\circ}10'\) (1)
- \(b = 1.2858\) (3) nm  \(\beta = 115^{\circ}57'\) (1)
- \(c = 1.4170\) (3) nm  \(\alpha = 91^{\circ}13'\) (1)

were obtained by least squares refinement of the centering.
parameters of eleven strong diffractions with $2\theta$ (Mo$_{\text{K}a}$) greater than 50° on a Picker FACS-1 automated diffractometer. This material plots on the $a^* - \gamma^*$ curve for low-temperature plagioclase of Smith (6, Figure 1).

The crystal structure of this plagioclase was refined from 9393 symmetry-independent X-ray diffraction intensities of which 5142 were greater than three times the standard deviations of the background count. Using isotropic thermal parameters for Si, Al, and O and anisotropic thermal parameters for Ca and Na, a minimum weighted residual of 0.048 for all data was obtained from a model containing a ten percent vacancy in one of the large cation sites, A(000) (notation of Megaw (7)). A split-atom model was required to fit the A(ZiO). Fractional coordinates of the two halves of the A(ZiO) site differ by as much as 100σ with negligible correlation coefficients between corresponding parameters of the two positions. The best fit of the data was obtained with the two halves of the A(ZiO) fully occupied by Ca, with 9 percent Na in each of the A(0i0) and A(Z00) positions and a 10 percent vacancy in the smallest A site, A(000).

This analysis is consistent with the prediction of Schwantke (8) and the conclusion of Grundy and Ito (9) for Sr feldspar, in that vacancy in the A-site is a major cause of non-stoichiometry in feldspars. Because the vacancy appears to be on the smallest A-site, it is possible that some of the vacancy is the result of subsolidus reduction of Fe$^{2+}$ which was ordered into the A(000) site. Such a mechanism would account for the blebs of Fe metal in the feldspar as described by Gooley et al. (1).

References


REFINEMENT OF ANORTHITE

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