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Crystal structure of iwakiite

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A small single crystal of iwakiite, $Mn(Fe,Mn)_2O_4$, from the Gozaisho mine, Fukushima Prefecture, Japan, (description by Matsubara et al., 1979) was investigated by X-ray film methods and the crystal structure was refined using a four-circle X-ray diffractometer. The crystal structure of iwakiite is that of a spinel which shows a weak tetragonal distortion. This distortion is assumed to be caused, in analogy to hausmannite, Mn_3O_4 , by Jahn-Teller effect of trivalent manganese.

Table 1. Crystallographic data and interatomic distances.

Space group: I4 ₁ /amd		
a = 6.025(1) A	Mn-O 2.025(2) A 4	x
c = 8.539(1) A	(Fe,Mn)-O 2.032(1) A 4	x
Z = 4	(Fe,Mn)-O 2.036(2) A 2	x

Weissenberg photographs of single crystals of iwakiite show additional reflections which might arise from an oriented intergrowth with manganosite, MnO. Even though the intensities of the strongest of these reflections are approximately 10 % of the strongest of iwakiite, a polished sample observed by ore-microscopy appears to be completely homogenous.

A microprobe analysis of iwakiite showed that at least 40 % of the cations are Fe atoms. If the existence of submicroscopic MnO is real the Fe content of pure iwakiite is even higher. This could explain the extremely weak Jahn-Teller distortion.

Literature

Matsubara, S., Kato, A., Nagashima, K.: Min. Journal <u>9</u>, 383-391 (1979).