

A COMBINED IN-SITU X-RAY AND MÖSSBAUER STUDY
OF THE $P2/n \leftrightarrow C2/c$ PHASE TRANSITION IN OMPHACITE $(\text{Na,Ca})[\text{Al,Mg,Fe}^{2+}]\text{Si}_2\text{O}_6$

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At intermediate compositions of the pyroxene solid solution jadeite $\text{NaAlSi}_2\text{O}_6$ - augite $\text{Ca}(\text{Mg, Fe}^{2+})\text{Si}_2\text{O}_6$ and at low temperatures an ordered phase with the space group $P2/n$ occurs, which is known as the mineral omphacite. In addition, natural omphacites may contain variable amounts of acmite $\text{NaFe}^{3+}\text{Si}_2\text{O}_6$. At temperatures around 860°C, the $P2/n$ omphacite undergoes a phase transition to the $C2/c$ space group which is caused by increasing cation disordering (see [1] and references therein). The space group $P2$ has also been described for the ordered omphacite [2]. In the $P2$ structure, there are four distinct M1 and four distinct M2 sites whereas in the $P2/n$ structure there are two distinct M1 and two distinct M2 sites. Structure refinements of the $P2/n$ omphacite show that Mg^{2+} and Al^{3+} are strictly ordered between the two kinds of M1 sites and that Na and Ca are partially ordered between the two kinds of M2 sites. Mg and Al alternate in successive M1 octahedra parallel to the c-axis. This ordering is mainly caused by the different ionic sizes and charges of Mg^{2+} and Al^{3+} as well as by their presence in approximately equal amounts. This ordering at the M1 sites is combined with an ordering at the M2 sites, i.e. Na^+ prefers the M2 sites close to Al^{3+} and Ca^{2+} the M2 sites close to Mg^{2+} in order to achieve local charge balance. An ideal formula for an ordered omphacite would be $(\text{Na}_{0.5}\text{Ca}_{0.5})[\text{Mg}_{0.5}\text{Al}_{0.5}]\text{Si}_2\text{O}_6$, i.e. $\text{Jd}_{50}\text{Di}_{50}$. In the present investigation a natural omphacite from the island of Syros, Greece is used [3]. Its structure and composition are determined by electron microprobe, scanning electron microscope, and single crystal X-ray diffraction. The transition temperature and the nature of the phase transition are determined by in-situ high temperature X-ray powder diffraction in treated and untreated samples under Argon and vacuum. In addition, heating experiments under controlled oxygen fugacities were performed with the same sample below and above phase transition temperature. The oxidation state and site distribution of iron in treated and untreated samples of both phases have been determined by Mössbauer spectroscopy. At present time, in-situ high temperature Mössbauer measurements are carried out.

Literature

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