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Local structure in *C*2/*c* clinopyroxenes on the hedenbergite ($CaFeSi_2O_6$)-ferrosilite ($Fe_2Si_2O_6$) join: A new interpretation for the Mössbauer spectra of Ca-rich *C*2/*c* clinopyroxenes and implications for pyroxene exsolution

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Abstract

Three synthetic Ca-rich clinopyroxenes on the hedenbergite-ferrosilite join, with compositions ($Hd_{50}Fs_{50}$), ($Hd_{60}Fs_{40}$), and ($Hd_{70}Fs_{30}$), were investigated by single-crystal X-ray diffraction and Mössbauer spectroscopy at room temperature. For all samples, there is no evidence for the presence of phases with symmetry other than *C*2/*c*. Structure refinement, using a split-atom model, shows the existence of two different local configurations in the M2 cavity, a hedenbergite-like arrangement and a *C*2/*c* clinoferrosilite-like arrangement that are centered by Ca and Fe^{2+}, respectively. The Mössbauer spectra were analyzed by a quadrupole splitting distribution (QSD) method, and the hyperfine parameters of the QSD fit indicate the presence of Fe^{2+} in three local environments that are similar to those of Fe^{2+} at the M1 site in hedenbergite, and the M1 and M2 sites in *C*2/*c* clinoferrosilite, in agreement with the structure-refinement results. Our results are consistent with the calculated phase diagram for hedenbergite-ferrosilite, where a miscibility gap and a two-phase field of metastable hedenbergite and metastable pigeonite occur at low temperature. The coexistence of a hedenbergite-like configuration around Ca and a *C*2/*c* clinoferrosilite-like configuration around Fe can be considered as a precursor for pyroxene exsolution at low temperature. Our results support previous structure-refinement work on Ca-rich clinopyroxenes along the diopside-enstatite join, and provide a new insight in the interpretation of Mössbauer spectra of Ca-rich *C*2/*c* clinopyroxenes.

Keywords: Clinopyroxene, hedenbergite-ferrosilite, crystal structure, local structure, Mössbauer spectroscopy, X-ray diffraction