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SPINELS RENAISSANCE: THE PAST, PRESENT, AND FUTURE OF THOSE UBIQUITOUS MINERALS AND MATERIALS

Si-magnetite nano-precipitates in silician magnetite from banded iron formation: Z-contrast imaging and ab initio study†

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ABSTRACT

Si-bearing magnetite or silician magnetite is common in low- and high-temperature rocks. However, details about possible Fe-silicate or Si-Fe-oxide discrete phases/nano-precipitates were not available due to the limitations of conventional high-resolution TEM. Combining Z-contrast imaging and ab initio calculation using density functional theory (DFT) method, we have derived both composition and crystals structure of the discrete nano-precipitates within host magnetite. The nano-precipitates of Si-magnetite with composition of $[\square_{0.5}Fe^{2+}_{0.5}]^{VI}[Fe^{3+}]^{VI}Si^{IV}O_4$ or γ-$Fe_{1.5}SiO_4$ occur in silician magnetite from a banded iron formation from Western Australia. In the Si-magnetite precipitates, Si replaces Fe^{3+} in tetrahedral sites of the magnetite structure and vacancies are introduced in the octahedral Fe^{2+} sites. The Si-magnetite precipitates distribute along {111} of the host magnetite. Widths of the precipitates are even multiples of d_{111} of magnetite, such as $2d_{111}$, $4d_{111}$, and $6d_{111}$. Ordering of the vacancies in the Si-magnetite will result in symmetry of $P4_332$, which is a subgroup of $Fd\bar{3}m$ for magnetite. Stacking of Si-magnetite and magnetite (111) layers along the [111] direction also occur in magnetite. The nano-precipitates result from exsolution of Si-magnetite from the host silician magnetite at low temperature. The occurrence of the thin nano-precipitates within the magnetite host results from the minimization of interfacial energy between the precipitate and the host magnetite. Relatively high concentrations of aqueous silica and Fe-silicate complex species in pore fluid might enhance the incorporation of Si into the silician magnetite during crystallization of the magnetite.

Keywords: Si-magnetite, silician magnetite, banded iron formation, Z-contrast imaging, DFT