A crystallographic study of natural "hydrohematite" and "turgite"

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(in review) Peterson et al. have investigated the hydrothermal crystallization of akaganéite (β-FeOOH) and its transformation to hematite (Fe2O3) in heated aqueous solutions using in situ, time-resolved synchrotron X-ray diffraction. Rietveld analysis of the incipient crystals of secondary nanohematite yielded a refined occupancy for Fe of ~0.75. As the reaction proceeded, these refined occupancy factors systematically increased, asymptotically approaching unity in all cases. Thus, if charge balance was achieved by H+, then the composition of the first hematite nanocrystals was FeOOH rather than Fe2O3, suggesting that the akaganéite-hematite reaction was nearly isochemical.

In the present study, the authors searched for crystallographic evidence that natural hematite can exhibit similarly high levels of Fe vacancies. Breithaupt (1847) introduced the term "hydrohematite" to describe an Fe hydroxide from Bavaria similar to hematite but with a water content half that of goethite. Hermann (1844) reported the same hybrid composition for an iron oxide he labeled "turgite". Brush and Rodman (1867) described similar Fe hydroxides from localities in the eastern United States. Both "hydrohematite" and "turgite" were discredited in the 7th edition of Dana's System of Mineralogy (Palache et al. 1944).

The U.S. National Museum of Natural History contains material labeled "turgite" from Hermann's type locality and hematite specimens from several of the U.S. localities described by Brush and Rodman (1867). Our X-ray diffraction and SEM analysis of the type "turgite" material from Turginsk revealed it as a glassy Fe silicate with minor inclusions of hematite and goethite in roughly equal amounts. In contrast, our Rietveld analysis of "turgite" specimens from Connecticut (donated by Brush) yielded a hematite structure with a refined Fe occupancy of ~0.84. Specimens from Pennsylvania and Virginia offered similar results. Thus, natural crystals of hematite can contain high concentrations of Fe vacancies due to the incorporation of water in amounts that approach those found in goethite and akaganéite.