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A neutron powder diffraction study of Fe and Ni distributions in synthetic pentlandite and violarite using ^{60}Ni isotope

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ABSTRACT

Cation ordering in two important iron nickel sulfide minerals, pentlandite and violarite, was studied by neutron powder diffraction using samples prepared with isotopically enriched ^{60}Ni. Pentlandite of composition $Fe_{4.8}Ni_{4.2}S_8$, annealed at 150° C for 1 month has a disordered Ni/Fe distribution with Ni occupying 57(2)% of the octahedral site and 46(1)% of the tetrahedral site with a unit cell repeat of 10.1075(1) Å. After annealing for a further 2 months at 150 °C the Ni/Fe distribution is still disordered with 53(2)% Ni in the octahedral site and 48(2)% Ni in the tetrahedral site and the cell parameter increased by 0.21% possibly due to slight readjustment of the Fe/Ni ratio.

Synthetic violarite, $FeNi_2S_4$, prepared at 300 °C, exhibits ordering of Ni onto the tetrahedral site, with Fe and the remaining Ni sharing the octahedral site. In situ neutron diffraction heating experiments in which pentlandite and violarite were heated up to 300 °C for 12 hours did not alter the Ni/Fe distribution between tetrahedral and octahedral sites. Violarite did not exhibit any evidence of magnetic ordering upon cooling to –173 °C. The interatomic distances in the two structures indicate that in pentlandite Fe^{2+} and Ni^{2+} are high spin and in violarite Fe^{2+} is low spin with Ni^{3+} with an inverted spinel structural type.

Keywords: Neutron diffraction, cation ordering, ^{60}Ni isotope, pentlandite, violarite, thiospinel