American Mineralogist, Volume 83, pages 1045–1053, 1998

Cation sites in Al-rich $MgSiO_3$ perovskites

D. ANDRAULT,[1,]* D.R. NEUVILLE,[1] A.-M. FLANK,[2] AND Y. WANG[3]

[1]Laboratoire des Géomatériaux, IPGP, CNRS-ESA 7046, Paris 75252, France
[2]Laboratoire pour l’Utilisation du Rayonnement Electromagnétique, Orsay 91405, France
[3]CHIPR, State University of New York, Stony Brook, New York 11794, U.S.A.

ABSTRACT

Local structure analysis of Al-containing magnesium silicate perovskite has been carried out with X-ray absorption spectra recorded at the Mg, Al, and Si *K*-edges using the SA32 beam-line of SuperAco (Orsay, France). The Al-XAFS spectrum of $(MgSi)_{0.85}Al_{0.3}O_3$ perovskite (synthesized in a multi-anvil apparatus) cannot be explained by assuming that Al^{3+} occurs in octahedral or dodecahedral sites only. This conclusion is based on comparison between Al-spectrum and those recorded at the Mg and Si *K*-edges for the same structure, general trends found for Al-spectra in various atomic sites, and ab-initio calculations using the FEFF-6 code. Thus, Al appears to be partitioned between both octahedral and dodecahedral perovskite sites. However, the structural accommodations needed to stabilize Al^{3+} cation in such different sites are not straightforward. Also, Mg *K*-edge spectra in enstatite and perovskite were compared with those previously reported at the Fe *K*-edge for the same structures, confirming that these two elements are located in the same polyhedra in both structures, and thus that Fe^{2+} enters the dodecahedra of the silicate perovskite.