

XAFS spectroscopic study of Ti coordination in garnet

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ABSTRACT

Titanium can be incorporated either tetrahedrally (^{IV}Ti) or octahedrally (^{VI}Ti) in most silicate minerals. Ti *K*-edge X-ray absorption fine structure (XAFS) spectroscopy enables observation of Ti coordination in minerals and melts. In this study, XAFS is used to determine the coordination of Ti in synthetic and natural garnets. Garnets grown synthetically at eclogite- and granulite-facies conditions can contain several wt% TiO₂, most of which is incorporated as ^{VI}Ti. This observation aligns with major element trends in these garnets. In natural garnets grown at lower temperatures and pressures, on the other hand, Ti is observed to occupy both the octahedral and tetrahedral sites in garnet—in some cases Ti is almost entirely fourfold coordinated. Combined with previous research (see Ackerson et al. 2017, this issue) on substitution mechanisms for ^{VI}Ti, the results of this study demonstrate that Ti is incorporated on two crystallographic sites in garnet by at least three primary substitution mechanisms. In both natural and synthetic garnets, there is a discernible increase in ^{VI}Ti content in garnet with increasing temperature and pressure, suggesting a significant role for these two parameters in determining Ti solubility. However, a continuous increase in ^{VI}Ti with increasing grossular content also suggests that the Ca content of the garnet plays a critical role.

Keywords: Garnet, Ti substitution, XANES, XAFS