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# Ti site occupancy in natural and synthetic zircon.

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Since the development of the titanium in zircon thermometer, it has become a well utilized tool to explore zircon re/crystallization on Earth. Its usefulness has also been extended to extraterrestrial settings including lunar and eucrite samples [1,2]. With Ti in terrestrial systems being largely expected to be tetravalent, the possibility of Ti substituting into either the tetravalent Si (4-fold) or the tetravalent Zr (8-fold) site in zircon were both considered plausible [3]. Some insight into this question was placed on firmer ground with new thermodynamic models and Ti XANES spectra that identified the Si site in synthetic zircon as the primary location for Ti [4,5]. Based on results from laboratory experiments, the model equilibrium reaction involves an exchange of Ti4+ for Si4+ in the zircon structure (i.e., $TiO_2 + ZrSiO_4 = SiO_2 + ZrTiO_4$). To explore this further we collected Ti XANES spectra on terrestrial, extraterrestrial, and laboratory synthesized zircon. The laboratory experiments were conducted under titania- and silica-activity buffered conditions; in all cases the titania activity was fixed at 1 whereas the silica activity was buffered at different values. Our preliminary results show that the variation of Ti distribution between Si and Zr sites of natural and experimental zircon is larger than previously expected, with a sometimes-significant fraction of Ti detected in the 8-fold Zr site. While our preliminary assessment is that this observation will be unlikely to significantly impact temperature estimates based simply on measuring the Ti concentration in zircon, it demonstrates that XANES spectra of natural zircon have the potential to reveal and track intensive variables previously unrecognized. For instance, future study will explore the role of silica activity in the system and the speciation of Ti in zircon.

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