MS15-03 | The True Structural Relationship between Zicon and Scheelite Structure Types, and a New Polymorph of Zircon

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Zircon ($ZrSiO_4$, $I4_1/amd$) is a very common accessory mineral and important ceramic component. Its high-pressure polymorph with a scheelite-type structure, reidite ($I4_1/a$), has been detected in impact structures where it is diagnostic of shock impacts. Because $I4_1/a$ is a sub-group of $I4_1/amd$ many authors have assumed that reidite (and scheelite structures in general) can be obtained by a displacive-type distortion of the zircon structure. Careful analysis of the atomic linkages and symmetry elements in the two structure types shows that this is incorrect, and that the transformation between them must be reconstructive and first order. This is consistent with survival of reidite in meteorite craters, and confirmed by our new ab-initio DFT simulations [1].

The DFT simulations also revealed that zircon has a soft phonon mode that triggers a displacive transition near 20 GPa to a previously-unreported $ZrSiO_4$ phase with symmetry I-42d. We have confirmed the occurrence of a soft-mode driven second-order phase transition by in-situ high-pressure Raman spectroscopy [2]. This also showed that reidite starts to form in the sample just after the transition to the new phase. Thus, at room temperature, the first-order activation barrier between zircon and reidite can be overcome via the formation of the new high-pressure phase as an intermediate bridging state.

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[1] Stangarone et al. (2019) American Mineralogist, doi: 10.2138/am-2019-6827
[2] Mihailova et al. (2019) Physics & Chemistry of Minerals, submitted