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In situ HT-XRD Study of Zircon - Tackling Inconsistencies in Thermal Expansion Data

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Information on the fundamental structural properties of zircon ($ZrSiO_4$) under high temperature conditions is surprisingly scarce and partially inconclusive. Moreover, there have been some observations of anomalies in structural and related thermal expansion data from *in situ* neutron powder diffraction experiments [1], which became interpreted as to indicate a displacive phase transition in high temperature zircon [1, 2]. Accordingly, a phase transition could, for instance, potentially compromise the extrapolation of experimentally determined high temperature zircon properties to notably lower temperatures, such as trace element distribution and solubility data applied to aid the petrologic interpretation of the U-Pb zircon geochronometer. For such reasons, we aimed to probe for the alleged zircon phase transition.

HT-XRD experiments have been performed on powdered zircon samples, using an Anton Paar HTK 1200 furnace attached to a Philips X'PERT-MDP equipped with a primary beam Ge-(111) monochromator (Cu Kα_1 radiation). Diffraction data was collected for heating steps along complete temperature cycles between room conditions and 1150˚C. Investigated samples comprise two groups: (a) various fully crystalline or now near-to-completely annealed, previously radiation damaged natural zircons, as well as synthetic (Zr,Y)(Si,P)O_4 zircon solid solutions; (b) significantly radiation damaged natural zircon. Lattice parameters at room temperature were determined as characteristic for the respective structural state and chemical composition.

Heating the crystalline (group a) zircon samples from room temperature to 1150˚C, *in situ* lattice parameters monotonously increased with increasing temperature in such a manner that the axial ratio a/c linearly decreased. Lattice parameters determined along both limbs of the complete cycle (heating and cooling back to room temperature) followed the same path. The slope of the axial ratio a/c was similar for all investigated crystalline samples and notably constant within the explored temperature interval. The complete heating cycle of radiation damaged zircon (b), however, described a hysteresis loop: the resulting axial ratio slope was kinked and, due to annealing at high temperature, the *in situ* lattice parameters became identical to those of the crystalline samples.

Our experiments have been cycled across the temperature of $\sim$ 827˚C, at which a previous study [1] observed a significant anomaly of structural properties during heating of their zircon sample. Our heating cycle of radiation damaged zircon exactly replicated those findings. In addition, no anomaly in the temperature dependence of lattice parameters could be detected for the various crystalline zircon samples investigated here. In conclusion, thermal expansion data bears no evidence on a displacive phase transition in HT zircon. Up to the dissociation temperature, no phase boundary is crossed and zircon is indeed a single phase. New results allow to compile a consistent data set of zircon thermal expansion properties.

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