An X-ray diffraction and structural refinement study of radiation-damaged zircons from Bancroft, Ontario

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Powder X-ray diffraction (XRD) is one of the most fundamental analytical tools used to characterize materials. Minerals, rocks, high-temperature superconductors, fullerenes, and magnetoresistance devices are examples of materials for which powder XRD has had a major impact in understanding their structures and in their technological development. The main objective of this study is to investigate using powder XRD what happens to extremely metamict (i.e., extremely radiation damaged) zircon ($ZrSiO_4$) crystals from Bancroft, Ontario, when subjected to high temperature (e.g., 800–1200°C) annealing over extended periods of time (up to 36 hours) and what materials are made as part of that process. The X-ray data collected will be compared to known structures of zircon, monoclinic and tetragonal ZrO_2, polymorphs of SiO_2, and potential U, Th, and Pb phases that might be part of the breakdown of zircon during metamictization and that may form during the recrystallization process.

The main reason this study was undertaken was to obtain a better understanding of what physically happens to zircon in the CA-TIMS (chemical abrasion - thermal ionization mass spectrometry) method for treating single zircon crystals before U-Pb TIMS isotopic age measurements are made. So-called waterfall plots of the XRD data have been made using the JADE software program, and further detailed plots will be made in IgorPro, a scientific graphing program, to show the effects of the annealing and recrystallization as a function of time and temperature. The data suggest that during the annealing process, zircon recrystallizes and also tetragonal ZrO_2 and SiO_2 phases are formed. These phases will be further quantified using transmission election microscopy (TEM) to determine the structure of the SiO_2 phase and to determine if the ZrO_2 is only tetragonal ZrO_2 or if monoclinic ZrO_2 (baddeleyite) is also present.

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