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# Reexamination of the structure of nanomineral opal-CT using synchrotron X-ray diffraction, transmission electron microscopy, X-ray scattering structure factor, and pair distribution function analyses

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## Abstract

Nanomineral opal-CT is a natural precursor to quartz formed by various geological processes, including weathering, biological precipitation, hydrothermal alteration, and shock metamorphism. These processes play a crucial role in the formation of siliceous rocks as well as abiotic and biogenic interactions in natural systems. Hydrous opal-CT was recently found on the surfaces of Mars and the Moon by microanalyses and remote sensing, which has led to further investigation into the characteristics of opal-CT. In this work, we have investigated the local structures of natural opal-CT samples with various degrees of crystallinity using a combination of synchrotron X-ray diffraction (XRD), X-ray scattering structure factor $S(Q)$ analysis, transmission electron microscopy (TEM), and pair distribution function (PDF) analysis. The combined results indicate that opal-CT is mainly composed of interstratified tridymite and cristobalite nanodomains with twins and stacking faults. $S(Q)$ patterns are used to delineate the XRD data of opal-CT samples, which provide more precise peak profiles, allowing for better determination of the degree of ordering. TEM images and selected-area electron diffraction (SAED) patterns directly show nanodomain structures with planar defects. X-ray PDF analysis is a powerful characterization tool that can further unveil local structures, defects, and crystallinity in opal-CT. The rise in ordered domain size and two peaks at 10.01 and 11.16 Å in G($r$) plot reflect the increase in the amount of cristobalite units and crystallinity. Both four- and eight-membered [$SiO_4$] rings are created by twinning and stacking faults of the tridymite and cristobalite domains. X-ray PDF analysis provides unique insights into the local structures, crystalline sizes, and ordering degree of opal-CT. Quantifying the crystallinity of natural opals is important to understanding the diagenetic processes of opals and the associated diatomaceous clays in sedimentary formations.

**Keywords:** Opal-CT, nanomineral, mineraloid, synchrotron X-ray diffraction, X-ray scattering structure factor, transmission electron microscopy, pair distribution function analysis