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First in situ X-ray identification of coesite and retrograde quartz on a glass thin section of an ultrahigh-pressure metamorphic rock and their crystal structure details

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Abstract

To ensure the presence of coesite and its transformed polymorph, quartz, in ultrahigh-pressure (UHP) rocks and to examine the relic of the phase transformation, crystal structures were analyzed by single-crystal X-ray diffraction (XRD) directly using the rock thin section mounted on a slide glass. The rock sample used is a coesite-bearing eclogite from the Sulu UHP terrain, eastern China. The crystal structures were determined successfully by this new method and the presence of coesite and quartz in UHP rocks was identified for the first time by XRD. The *R*-factor [*R*(*F*)] converged to 0.046 for coesite and 0.087 for quartz. The displacement ellipsoids for coesite and quartz are larger than those previously reported for these two phases, which is consistent with expected effects of trapped strain due to the phase transformation from coesite to quartz during exhumation from the Earth's mantle.

This paper is the first report of single-crystal XRD of a rock thin section on a glass slide and establishes the technique, and provides proof-of-concept of the method. Although the mineral species included in a thin section can often be identified by other methods, such as Raman spectroscopy, an advantage of the reported method is that it can be applied to any mineral in a thin section, and not just to the UHP minerals. Moreover, it is applicable to an unknown or new mineral in a thin section, discarding the spots of known minerals and constructing a lattice from the residual spots to find the structure of the unknown phase.

Keywords: Crystal structure, coesite, quartz, UHP rock, thin section, XRD, displacement ellipsoid