Geophysical Research Abstracts, Vol. 7, 10957, 2005
SRef-ID: 1607-7962/gra/EGU05-A-10957

High pressure powder neutron diffraction of thorite ($ThSiO_4$)

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Thorite and huttonite are the two known phases of $ThSiO_4$ that occur naturally, but natural samples are commonly metamict due to the presence of thorium. Thorite is tetragonal $I4_1$/*amd* with $a = b$ = 7.1328(2) c = 6.3188(2). Huttonite is monoclinic, $P2_1/n$ with a = 6.784(2) b = 6.974(3) and c = 6.500(3) β =104.99° and isostructural with monazite, a more common phosphate mineral. Specimens of thorite generally come from igneous pegmatites and volcanic extrusive rocks, hydrothermal veins and contact metamorphic rocks as well as small grains found in detrital sands.

The high resistance and stability of zircon in upper mantle conditions have made the monazite structure minerals an interesting group to look at in the high-pressure community. While zircon has been extensively studied at high-pressure, data are lacking for thorite and huttonite. Because thorium is a strong x-ray scatterer (unlike Si and O), the use of neutron scattering provides better contrast and makes it easier to obtain accurate atom positions for Si and O.

Since natural samples of thorite are commonly metamict and often occur in association with uranium, we have synthesized $ThSiO_4$ for this experiment. The sample was made with a sol-gel hydrothermal synthesis technique from $Th(NO_3)_4$* $4H_2O$ and $SiHCl_3$ at 220^{o}C for 10 days. Thorite can be converted irreversibly to huttonite by heating at 1200 ^{o}C in air for a few hours.

Our study of the thorite sample at the Los Alamos Neutron Science Center uses a large volume moissanite (SiC) anvil cell. The moissanite anvils are weakly absorbing and provide higher neutron flux to the sample than is possible with tungsten carbide anvils. The diffracted beam intensities are obtained by integrating the detected intensities from 192 ^{3}He tubes, arranged in eight panels around the beam direction at a diffraction angle of 90^o. We will describe the mechanical properties of thorite at high-pressure and will discuss the possibility of a pressure-induced phase transition from thorite to huttonite. As well as the possible dissociation into ThO_2 and SiO_2 at very high pressures. (Reidite dissociates into ZrO_2 (cotunnite) and SiO_2(stishovite) at about 20 GPa (Tange and Takahashi, 2003) and since they are isostructural, thorite should follow a similar transition.) We will also compare our neutron measurements at high-pressure with x-ray diffraction and Raman data.

Tange, Y., Takahashi, E. (2003): Stability of high-pressure polymorph of zircon ($ZrSiO_4$) in the deep mantle. Physics of the Earth and Plantary Interior.