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Report:

The high-pressure behavior of kyanite, Al_2SiO_5, has been discussed controversially for several years, where both a disproportionation into its oxide components corundum (Al_2O_3) and stishovite (SiO_2) [1,2] and the occurrence of a new high-pressure polymorph with V_3O_5-like structure [3] have been proposed. As the possible occurrence of a new high pressure polymorph would have significant geophysical implications, we wanted to check the existence of this new phase and to provide physical and chemical data, which are essential to estimate the possible role of Al_2SiO_5 in the deep earth.

Our investiagtions on the high-pressure behavior of both sillimanite (another Al_2SiO_5 polymorph) and kyanite were carried out by means of powder X-ray synchrotron diffraction, a Bruker SMART CCD detector and a diamond-anvil cell as a pressure-generating device. Maximum pressures of 46 and 53 GPa, respectively, were produced. Unit-cell parameters were refined and allowed a fit to a second-order Birch-Murnaghan equation of state. The bulk moduli of sillimanite and kyanite obtained are B_0 = 176(11) GPa and B_0 = 190(3) GPa at fixed B' = 4, respectively. This is in reasonable agreement with previously published data, e.g., [4, 5]. The samples were laser annealed several times at high pressures. After laser annealing at 46 GPa, sillimanite was found to have decomposed into its oxide components corundum and stishovite. The high-pressure behavior of kyanite, however, is more complicated. Up to 20 GPa, kyanite remains stable. At 30 GPa a new high-pressure form is observed, which seems to be structurally related to kyanite. We deduce this from the appearance of 5 additional peaks (Figure 1). After laser heating, partial disproportionation into corundum and stishovite was observed. However, when laser heating at much higher pressures of 47 to 53 GPa, the new phase remained stable. In summary, our results indicated that both disproportionation and a phase transformation, depending on the applied *P-T* conditions, may occur. However, the previously reported monoclinic unit cell [3] is inconsistent with our data. The results obtained here are promising but tentative. We are now confident, that the controversial discussion can be resolved by collecting higher quality data, which could be achieved by laser-heating the sample from both sides in a better controlled way.

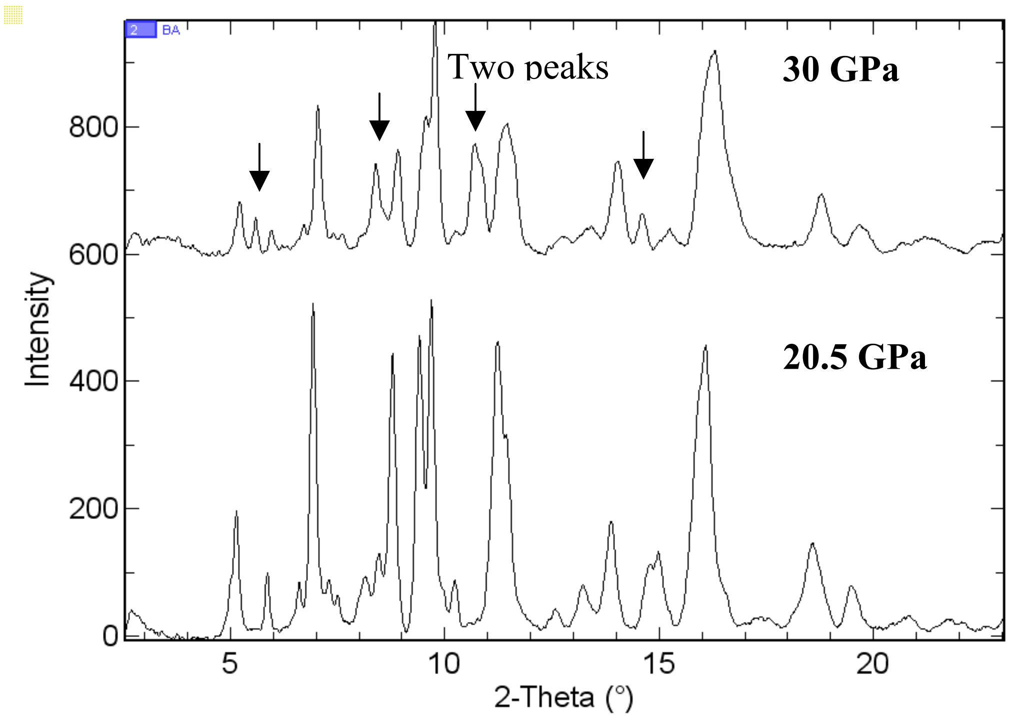

Figure 1. X-ray synchrotron powder diffraction patterns of kyanite (at 20.5 GPa) and the new high-pressure polymorph (at 30 GPa) after subtraction of the background intensity using a Chebychev function. The pattern at 30 GPa was offset by 600 in vertical direction in order to enable a better comparison. The new peaks are marked by black arrows.

Literature:

[1] Liu, L.-G. (1974) Earth and Planetary Science Letters, 24, 224 – 228.

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[3] Ahmed-Zaid, I. and Madon, M. (1991) Nature, 353, 426 – 428.

[4] Yang, H., Downs, R.T., Finger, L.W., Hazen, R.M., and Prewitt, C.T. (1997) American Miner., 82, 467 – 474.

[5] Yang, H., Hazen, R.M., Finger, L.W., Prewitt, C.T., and Downs, R.T. (1997) Phys. Chem. Minerals, 25, 39 – 47.