The Compression Behavior of Ca(OH)2 Portlandite

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Portlandite Ca(OH)₂ is a member of the family of brucite-type simple hydroxides. It has a very anisotropic layered structure based on close-packed octahedral CaO_6 layers separated by hydrogen in the interlayers. The weak interactions at the interlayers result in a large elastic anisotropy, close to 60% of the Young's modulus at ambient conditions. The study of the high-pressure behavior of portlandite is appealing in different respects. Portlandite is a model system to investigate the effect of hydrogen incorporation in simple oxide structures; in addition, it is considered a prototype of that class of materials that are subject to pressure-induced amorphization. A very recent study (Catalli and Shim, 2007) shows that the previously proposed (Meade and Jeanloz, 1990) pressure-induced amorphization of $Ca(OH)_2$ at P > 11GPa could be due to structural disordering induced by large non-hydrostatic stress conditions in previous high-pressure experiments. Another important result of that study is that Ca(OH)₂ undergoes a polymorphic transition at pressures above 8 GPa. In order to assess both the intrinsic pressure dependence of the elastic properties of portlandite and its high-pressure stability, we have performed synchrotron x-ray powder diffraction experiments in different compression devices and different pressure transmitting environments (large volume press in NaCl pressure medium and diamond anvil cell in Ar medium) up to 12.5 GPa at ambient temperature and we have also directly determined its single-crystal elastic tensor by Brillouin spectroscopy at ambient conditions. In our high-pressure experiments we do not detect any polymorphic transition. Based on our results, we confirm that the apparent pressure-induced amorphization is indeed a result of nonhydrostaticity, as demonstrated by the contrasting results of our experiments performed in NaCl pressure medium (total disappearance of the x-ray diffraction lines at P > 11 GPa) with respect to those performed in a softer Ar pressure medium (persistence of the diffraction lines up to 12.5 GPa). In addition, the unit-cell parameters determined from x-ray diffraction of portlandite powder at high pressures could be biased as a result of the unusually large elastic (and plastic) anisotropy of this mineral, poor sampling of the reciprocal space, and specific details of the local stress environment that are caused by the design of the different compression devices and pressure transmitting media. References

Catalli K, Shim S-H, and Prakapenka VB (2007) A crystalline-to-crystalline phase transition in Ca(OH)2 at 8 GPa and room temperature. Geophys Res Lett 35: L05312

Meade C, and Jeanloz R (1990) Static compression of Ca(OH)2 at room temperature: Observation of amorphization and equation of state measurements to 10.7 GPa. Geophys res lett 17: 1157-1160

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