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The structural phase transformations in the chalcopyrite semiconductor AgInTe₂ have been studied up to 10 GPa on both pressure increase and decrease. The experiment were carried out using angle-dispersive X-ray diffraction with synchrotron radiation and an image plate. The diffraction patterns of AgInTe₂ at ambient pressure reveal two coexisting phases: the first has the chalcopyrite structure while the second has a zinc blende like structure. On pressure increase both phases transformed at 3-4 GPa to a cation-disordered structure with spacegroup Cmcm, the atomic coordinates of which $v=0.75$ for Ag or In and $v=0.25$ for Te - correspond to a NaCl-like structure. On pressure increase the Cmcm phase was stable up to at least 10.25 GPa. On pressure decrease, the chalcopyrite phase started to reappear at 0.55 GPa, and the Cmcm phase disappeared completely at ambient pressure. In addition to the experimental study, we have also performed density functional theory calculations. The calculated transition pressure from the chalcopyrite phase to the Cmcm phase is 4.08 GPa, and the calculated atomic positions in the Cmcm phase are in excellent agreement with those determined experimentally.

Keywords: diamond anvil cells, X-ray diffraction, *ab-initio* calculations

P20.03.11

Acta Cryst. (2008). A64, C609

High-pressure behavior of iron-nickel phosphides and its implications for meteorites and Earth core

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Minerals with composition (Fe,Ni)_xP, are rare, but important accessory phases present in iron, and chondrite meteorites. The occurrence of these minerals in meteoritic samples is believed to originate either from the equilibrium condensation of protoplanetary materials taking place in solar nebulae or from crystallization processes in the cores of parent bodies. Fe-Ni phosphides are considered an important candidate for a minor phase present in the Earth core, and at least partially responsible for the observed core density deficit with respect to pure Fe. We report results of high-pressure high-temperature single-crystal X-ray diffraction experiments with a range of materials belonging to the (Fe,Ni)_xP family, including Fe₃P, Fe₂P, and Ni₂P. A new phase transition to the Co₂Si-type structure (allabogdanite) has been found in Fe₂P at 8.0 GPa, upon heating. The high-pressure phase can be metastably quenched to ambient conditions at ambient temperature, and then, if heated again, transforms back to barringerite. Contrary to the recent reports, we find Fe₃P to remain stable in the schreibersite structure up to at least 60 GPa and 2000 K. Our results indicate that the presence of allabogdanite in meteoritic samples places two important constraints on the thermodynamic history of the meteorite. First, it imposes a minimum pressure and temperature for the formation of the Fe₂P, and additionally rules out any higher temperature low pressure alterations. If present in the Earth core, Fe₂P will have the allabogdanite rather, than barringerite structure. Crystal chemical

trends in the compressibility and thermal expansion of (Fe,Ni)_xP compounds, as well as polymorphic transition paths are analyzed in the context of the Earth's core composition and properties.

Keywords: Earth core, phase transitions, high pressure

P20.03.12

Acta Cryst. (2008). A64, C609

High-pressure and low-temperature charge density study of Pr_{1-x}Ca_xCoO₃ by SR powder diffraction

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The Pr_{1-x}Ca_xCoO₃ system exhibits a phase transition from a conductive to an insulating state with decreasing temperature under high pressure. The transition has found in the very narrow region of $x \sim 0.5$ at ambient pressure. Similar transition has also found in the wide x region under high pressure. No indication of this kind of transition has been observed in other species of R and A in the R_{1-x}A_xCoO₃ system (R = rare earth elements; A = Ca, Ba and Sr). The structural change through the pressure-induced phase transition under high pressure has never been determined. To investigate the structural change and the role of Pr and Ca in the pressure-induced phase transition, we carried out the high-pressure and low-temperature structural study of Pr_{0.7}Ca_{0.3}CoO₃ by the synchrotron radiation (SR) powder diffraction. The phase transition from a conductive to an insulating state has been found above 1.0 GPa for Pr_{0.7}Ca_{0.3}CoO₃ by the electrical resistivity measurement. The SR powder diffraction data of Pr_{0.7}Ca_{0.3}CoO₃ were collected at Spring-8 BL10XU beamline. The sample pressure and the temperature were controlled by the He-gas flow type cryostat combined with a He-gas driven diamond anvil cell (DAC). A change of the diffraction pattern indicating the structural phase transition was observed around 100 K at 1.3 GPa. The electron charge density distributions and the crystal structures were determined by the MEM/Rietveld analysis. It was revealed that the covalency of Pr/Ca-O bond is increased in the low-temperature phase. This fact implies that the Pr 4f-O 2p orbital hybridization contributes to the stabilization of the low-temperature insulating phase.

Keywords: high pressure, charge density, Co oxides

P20.03.13

Acta Cryst. (2008). A64, C609-610

Synthesis and structure of new platinum hydrides at high pressure

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