Stability of the high pressure phase $Fe_3(S,O)_2$ to Earth and planetary core conditions in the Fe–S–O system

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Abstract

Cosmochemically abundant light elements, including S and O, are likely important alloying components in terrestrial planetary cores. Determining the thermodynamic properties of Fe-(S,O) alloys at high pressure and temperature further constrains the thermal and chemical structure of Earth and planetary cores. The high *P, T* subsolidus phase relations were determined in Fe–S–O alloy compositions to 177 GPa and 3300 K using synchrotron X-ray diffraction in a laser heated diamond anvil cell and chemical analyses of recovered samples by FIB/SEM. In sulfur and oxygen rich starting compositions, we report the stability of a *P*-type monoclinic $Fe_3(S,O)_2$ phase coexisting with *B*1-FeO and hcp-Fe to 60 GPa and $\sim$1900 K, above which it reacts with Fe to form Fe_3S. Above 80 GPa, a *P*-type monoclinic $Fe_3(S,O)_2$ phase is stable to 177 GPa and $\sim$2900 K with *B*1-FeO. Chemical analysis of a sample recovered from 40 GPa and 1570 $\pm$ 80 K reveals up to $\sim$15 atm% O solid solution into the $Fe_3(S,O)_2$ phase and confirms the coexistence of $Fe_3(S,O)_2$, FeO and Fe at these conditions. A recovered sample from 40 GPa and 1970 $\pm$ 80 K confirms the presence of FeO and Fe_3S and absence of $Fe_3(S,O)_2$ at high temperatures. The wide *P, T* stability field of these newly characterized $Fe_3(S,O)_2$ polymorphs indicate that they may crystallize in Fe, S, O-rich planetary cores.