Stability and phase diagram of solid and liquid Fe_xS_{1-x} alloys at conditions of the Earth`s core

KAREN VALENCIA[1], ALDEMAR DE MOYA[1], GUILLAUME MORARD[2] AND CARLOS PINILLA[1,3]

[1] *Departamento de Física y Geociencias, Universidad del Norte, Km 5 Via Puerto Colombia, Barranquilla, Colombia*

[2] *Institut de Mineralogie, de Physique des Materieux et de Cosmochimie, UMR CNRS 7590, Sorborne Universites – Universite Pierre et Marie Curie, 4 Place Jussieu, 75005, France.*

[3] *School of Chemistry, Bristol University, Bristol BS8 1TS, United Kingdom*

The observation of seismic waves, composition of meteorites, experimental and computational results of materials at extreme conditions indicate that the Earth's core (320 - 350 GPa and 5000-6500 K) is composed mostly of Iron (Fe) with a less presence of light elements such as S, Si or C, of high solubility at these conditions. The inclusion of these elements may explain the difference in density that exists between seismic data and relevant laboratory results. In this work, we have performed computational calculations based on functional density theory (DFT) to investigate the phase diagram for the Fe-FeS system at pressure and temperature conditions of the inner-outer core boundary. We have analised the stability, thermodynamic and structural properties of several liquid and solid solutions of FeS alloys ranging from a S concentration of 3.7wt% to 16wt%. We estimate sound velocities and show a collapse of magnetization after 50 GPa for most of the studied solid solutions. Additionally, we also have a look at the effect of S in the 54Fe/56Fe isotope fractionation at these conditions. Our results are discussed based on recent experimental observations and recent theoretical works.