Prediction of crystal structures and motifs in the Fe-Mg-O system at Earth’s core pressures

YANG SUN1, RENATA M. WENTZCOVITCH1, RENHAI WANG2, FENG ZHENG3, YIMEI FANG3, SHUNQING WU3, ZIJIN LIN2, CAI-ZHUANG WANG4 AND KAI-MING HO4

1Columbia University
2University of Science and Technology of China
3Xiamen University
4Iowa State University
Presenting Author: ys3339@columbia.edu

Fe, Mg, and O are among the most abundant elements in terrestrial planets. While the behavior of the Fe-O, Mg-O, and Fe-Mg binary systems under pressure have been investigated, there are still very few studies of the Fe-Mg-O ternary system at relevant Earth's core and super-Earth's mantle pressures. Here, we use the adaptive genetic algorithm (AGA) to study ternary Fe$_x$Mg$_y$O$_z$ phases in a wide range of stoichiometries at 200 GPa and 350 GPa. We discovered three dynamically stable phases with stoichiometries Fe$_5$Mg$_2$O$_6$, Fe$_2$MgO$_4$, and Fe$_3$MgO$_4$ with lower enthalpy than any known combination of Fe-Mg-O high-pressure compounds at 350 GPa. With the discovery of these phases, we construct the Fe-Mg-O ternary convex hull. We further clarify the composition- and pressure-dependence of structural motifs with the analysis of the AGA-found stable and metastable structures. Analysis of binary and ternary stable phases suggest that O, Mg, or both could stabilize a BCC iron alloy at inner core pressures.