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Fe-Mg phase equilibria under High-temperature and high-pressure conditions: experimental investigation and Calphad modeling

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Iron and magnesium are the object of many studies, in relation with the core/mantle chemical partitioning. Even if not directly applicable to geophysical environments, the phase equilibria within the Fe-Mg system at high-pressure and high-temperature represents an important end-member and is decisive for providing relevant thermodynamic modeling of more complex oxidized systems.

At ambient pressure, the Fe-Mg system shows complete immiscibility in solid state and a large miscibility gap in liquid state [1]. However, Dubrovinskaia et al. reported that solubility of magnesium in iron increases significantly with pressure, up to 7.8%at Mg at 89 GPa/3400°C [2]. Recently, ab-initio DFT calculations at 0K show the formation of Fe–Mg intermetallic compound under HP conditions [3] but they have not yet been experimentally confirmed.

The aim of the present work is to investigate Fe-Mg phase equilibria under HP-HT conditions to elucidate the occurrence of pressure-stabilized intermetallic phases as well as the evolution of mutual solubility of the two elements. Specific Fe-Mg samples, with a spontaneously organized bi-continuous microstructure of iron and magnesium, have been synthesized by dealloying process [4]. As the microstructure is formed from pure metals and within a Mg melt, it is also free of impurities and especially oxygen-free that is an important feature to study the binary system.

Experiments have been performed in Paris-Edinburgh press as well as in multi-anvil cells, up to 20 GPa and 1500K, with dedicated P-T cycles in order to avoid the formation of a liquid phase. Then, the final microstructure is carefully characterized (SEM-TEM+EDS, ICP-AES) and compared with the initial one. In parallel, gathered results are used to feed on going Calphad modeling of the Fe-Mg system including the pressure variable according to the formalism recently proposed by Brosh et al. [5].

References:

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