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Thermodynamics in the Fe-Si-O system up to 300 GPa

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The composition of the Earth's core in light elements such as Si, Mg, O or S, remains largely controversial. Conditions under which liquid metal saturates in these elements offer strong constrains on core composition. For instance, MgO can dissolve in the metallic phase at high temperature [1][2] and then precipitates upon core cooling. Similarly, exsolution of SiO_2 can occur if the liquid core start over saturated in Si and O and reach the saturation limit during secular cooling [3]. The issue of light elements exsolution/precipitation is crucial as it is a powerful source to drive the Earth's dynamo prior to inner-core growth.

We present a self-consistent thermodynamics approach that aims to determine the saturation conditions of liquid iron alloys in the Fe-Si-O system. The model is based on [5]. The Gibbs free energy of end-members are taken from [6] for Fe-liquid, Fe-HcP, Fe-Fcc, FeO-liquid, FeO-solid; [7] and [5] for stishovite and SiO_2-liquid; and [8] for FeSi-B2. We ran additional DFT calculations to constrain the EoS of SiO_2 liquid up to 300 GPa. The EoS of FeSi-liquid is extrated from [9] and a Gibbs free energy model for FeSi-liquid is fitted to match the FeSi melting curve of [10]. Activities in the liquid are fitted so that our model reproduces eutectic compositions and temperatures that have been measured experimentally in the Fe-Si-O system [e.g., 11,12,13].

We predict that SiO_2 precipitation in the Earth's core cannot occur for CMB temperature lower than 4300 K. This implies that it is unlikely that SiO_2 precipitation would have played a role in early Earth's dynamo. Moreover, our model indicates that SiO_2 precipitation would occur mostly in the upper outer core, i.e., P < 200 GPa.

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