MELTING IN THE FE-FES SYSTEM AND ITS RELATION TO THE COMPOSITIONS OF THE CORES OF EARTH AND MARS

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Thermal and physical evolution models of the cores of planetary bodies require knowledge of the physical and chemical characteristics of core-forming materials. Abundant evidence indicates that, although iron is the primary constituent of terrestrial planetary cores, there are lighter elements alloyed with the iron. In the past, models incorporating the effects of light elements have been hampered by a lack of data concerning the effects of these materials on the properties of iron at high pressures and temperatures.

This study makes use of recent melting curves of Fe [1] and FeS [2] at high pressures, combined with Fe-FeS eutectic data [3], to study the melting characteristics of the Fe-FeS system at high pressures. The melting curves o Fe and FeS are now well constrained at pressures characteristic of the earth' outer core (150 GPa) and data for the Fe-FeS eutectic composition and temperature are reported to 10 GPa. However, extrapolation attempts are hampered by phase changes in Fe and FeS below 5.5 GPa.

The melting model used here assumes ideal mixing of the end members in the melt and complete immiscibility in the solid state. It has been argued [4] that the Fe-FeS liquid solution may be nonideal, but the similarity in atomic radii between Fe and S, combined with the trend toward increasing ideality at low pressures [5], makes this unlikely. Arguments have also bee made [4] that FeS decomposes to Fe and FeS_2 at high pressure, but this is no seen upon static compression [6]. By analogy with low pressures [7], FeS is assumed to remain a distinct chemical species in the melt. This last assumption is less certain because the character of bonding in the Fe-S sys will change once S metallizes. Since this does not appear to affect the melting behavior of FeS [2], the effect is ignored in this treatment. With these assumptions, the parameters required for extrapolation of the liquidu are the melting curves of the two end members and the heats of solution, L_F and L_{FeS}, of the end members into the melt. A number of models for L were studied, but the one which agrees best with values derived from the eutect data [3] is a pressure-independent fit of the form $L = a + bT$, with $a_{Fe} = 13$ kJ·mol^{-1} and $b_{Fe} = -29$ J·mol^{-1}K^{-1}, and $a_{FeS} = 30$ kJ·mol^{-1} and $b_{FeS} = -41$ J·mol^{-1}K^{-1}.

Given a functional form for L, the liquidus can be calculated, using melting curves in Fig. 1, from

$$T = \frac{T_i}{1 + (RT_i \ln x_i / L_i)}$$

where T is the liquidus temperature, T_i is the melting temperature of pur R is the ideal gas constant, x_i is the mole fraction of i, and L_i is for liquidus temperature [8]. The resulting curves of T vs. P and x_S vs. P presented in Figs. 1 and 2, respectively. It should be noted that, abov GPa, these curves are very speculative because the eutectic occurs in th stability field of ε-Fe, whereas the eutectic data [3] on which the extrapolation is based is in the γ-Fe stability field.

The results of these calculations have several implications. The composition of the lowest-temperature liquids become more Fe-rich with increasing pressure at low pressures [9], but the present results show that this trend is reversed at higher pressures because of the divergence of the Fe and FeS melting curves. This indicates that previous extrapolations of the eutectic composition have sulfur contents much lower than those predicted here. Also, the relation of the extrapolated eutectic composition and liquidus temperatures can be compared to the estimated compositions of planetary cores at relevent pressures. Figures 1 and 2 indicate the pressures for the core-mantle boundary (CMB) and inner core boundary (ICB) of the earth and for the center of Mars (MARS). Also shown in Fig. 1 is the range of liquidus temperatures for the outer core of the earth (O. C.), based on the estimated sulfur content from [10]. The spread shown is due to the uncertainty in the composition of the core, rather than the uncertainty of the extrapolation. Applying appropriate error estimates, the minimum temperature at the CMB which would prevent feezing out of Fe is 4500±300 K, although the actual temperature can be anything above this value. The temperature at the ICB is constrained to be on the liquidus, since solid Fe and the melt coexist there. Thus, the ICB is expected to be at 7000±900 K. Figure 2 also presents the composition ranges (error bars at side) estimated for the earths outer core [10] and the core of Mars [11]. As can be seen, the reversal of the composition trend in the eutectic assures that the eutectic is more S-rich than the core of either planet.

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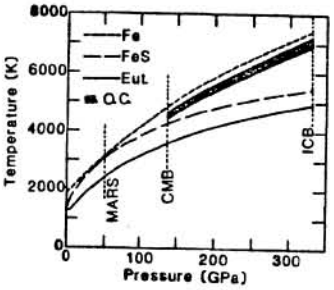

Fig. 1 - Melting curves.

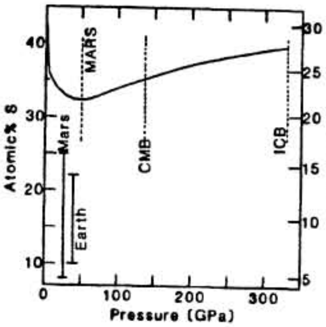

Fig. 2 - Eutectic composition.