# The effect of bulk composition on the behavior of sulfur during core formation

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## Summary

This investigation examines possible processes for core formation in chondritic bodies. Our model will inform the interpretation of geochemical data obtained from (16) Psyche. We find that the oxidation state of planetesimals affects their bulk and core compositions. Oxidized bodies make small S-rich cores and reduced bodies make large S-poorer cores.

## Purpose of study

In preparation for the NASA Psyche mission, we have modeled the partitioning of sulfur in primary chondritic planetesimal cores under a range of oxygen fugacities [1-3]. Sulfur is highly siderophile and immiscible in Fe-Ni liquid. It could make up a large part of a planetesimal core or form an immiscible sulfide liquid that could escape into the mantle, or potentially the surface of an exposed core [4]. We consider how the degree of melting of the planetesimal [1, 2, 6, 7] might affect the sulfur content of the core. If Psyche is a core or part of a core, which seems like the most likely scenario [5], we can predict potential sulfur contents of the core before impact stripping from its mantle if it formed from materials tested in this model.

## The model

Our model determines how sulfur partitions between the mantle and core of a planetesimal (eq. 1) with a range of starting chondritic compositions, which change with oxygen fugacity ($fO_2$). We used experimentally derived equations for $\log D_S$ (eq. 2) [2] and $\log C_S$ (eq. 3) [1]. The latter corresponds with oxygen fugacity ($fO_2$); low $\log C_S$ means the body is reduced, while high $\log C_S$ means that the body is oxidized [1, 2]. After finding $D_S$, we calculated the concentration of sulfur in the core of the parent body (eq. 4, 5) and the mass fraction of the core relative to the parent body (eq. 6). Enstatite and ordinary (H, L, LL) chondrites are considered reduced bodies and carbonaceous chondrites (CM, CI, CV, CO, CK) oxidized [10, 11]. The parent body's initial bulk sulfur and iron concentrations are determined from chondrite meteorite data (Table 1) [12]. Internal pressure is 0.1 GPa [3], and the temperature of partitioning is 1250˚C [7].

[eq. 1] $D_S = \frac{X_S^{core}}{X_S^{mantle}}$ [1, 2]

[eq. 2] $\log D_S = -3.30 + \frac{3000}{T} + 33 * \frac{P}{T} + \log X_{FeO}^{mantle} - \log C_S + 14 * \log(1 - X_O^{core})$ [2]

[eq. 3] $\log C_S = -5.705 + 3.15 X_{FeO}^{mantle} + 2.65 X_{CaO}^{mantle} + 0.12 X_{MgO}^{mantle} + 0.77 X_{TiO_2}^{mantle} + 0.75 (X_{Na_2O}^{mantle} + X_{K_2O}^{mantle})$ [1]

[eq. 4] $X_S^{core} = \frac{n_S^{core}}{n_{core}}$

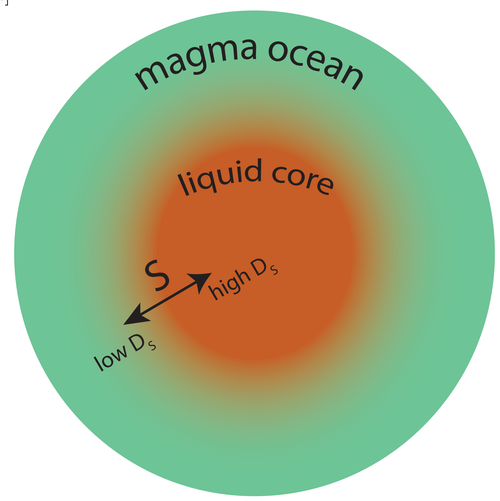
[eq. 5] $F_S^{core} = \frac{M_S^{core}}{M_{core}}$

[eq. 6] $F_{core}^{PB} = \frac{M_{core}}{M_{core} + M_{mantle}}$

Variable definitions:
$D_S$ = partition coefficient of S
X = mole fraction
T = temperature (K)
P = pressure (GPa)
$C_S$ = sulfide capacity of mantle
n = moles
M = mass
F = mass fraction

Table 1: Bulk chondrite metallic iron, FeO, and sulfur concentrations [data from 12].

| Chondrite | Fe (m) wt.% | FeO wt.% | S wt.% |
|---|---|---|---|
| En | 20.96 | 6.05 | 2.91 |
| H | 16.41 | 12.88 | 1.90 |
| L | 9.67 | 15.40 | 2.05 |
| LL | 5.99 | 17.30 | 1.94 |
| CI | 5.77 | 16.69 | 3.31 |
| CM | 4.55 | 22.78 | 2.58 |
| CO | 5.60 | 24.22 | 1.90 |
| CV | 2.99 | 24.44 | 1.20 |
| CK | 2.06 | 28.18 | 1.03 |




## Results

Figure 1

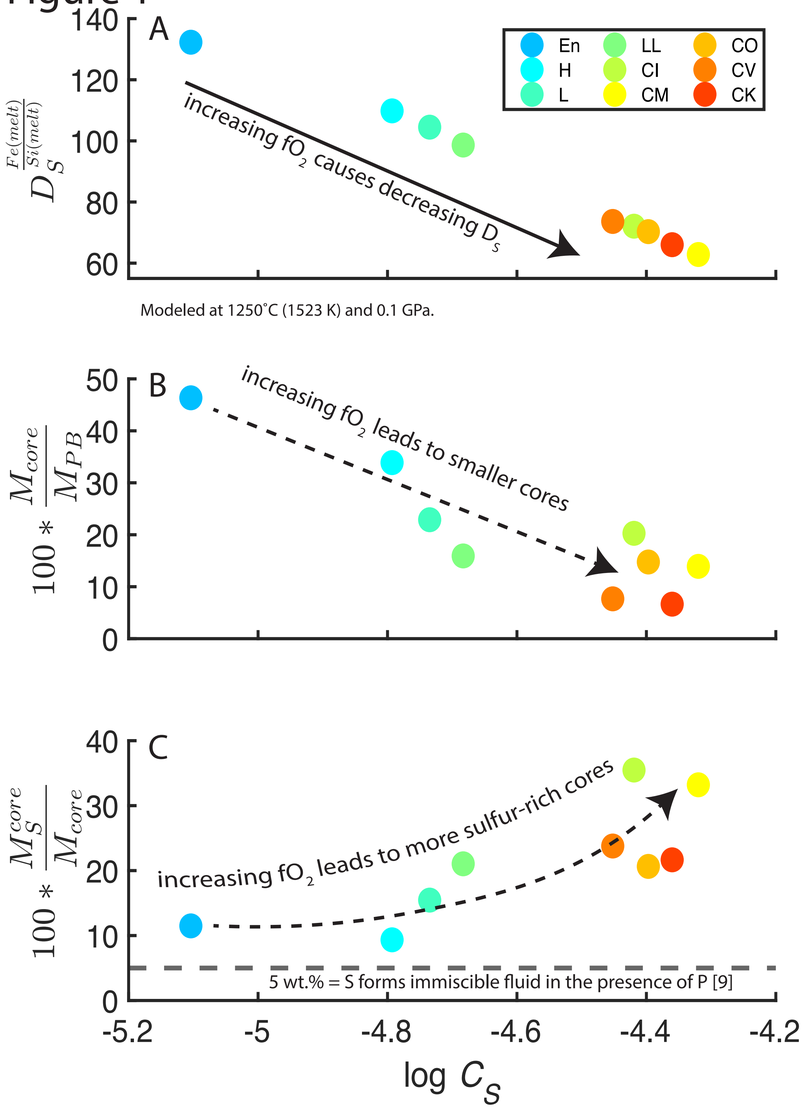
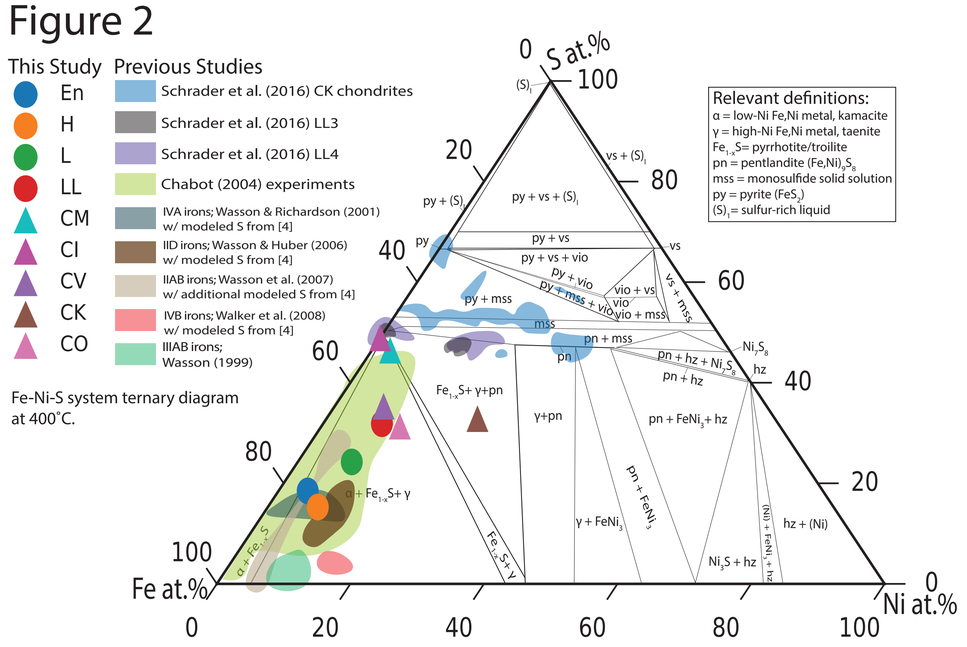


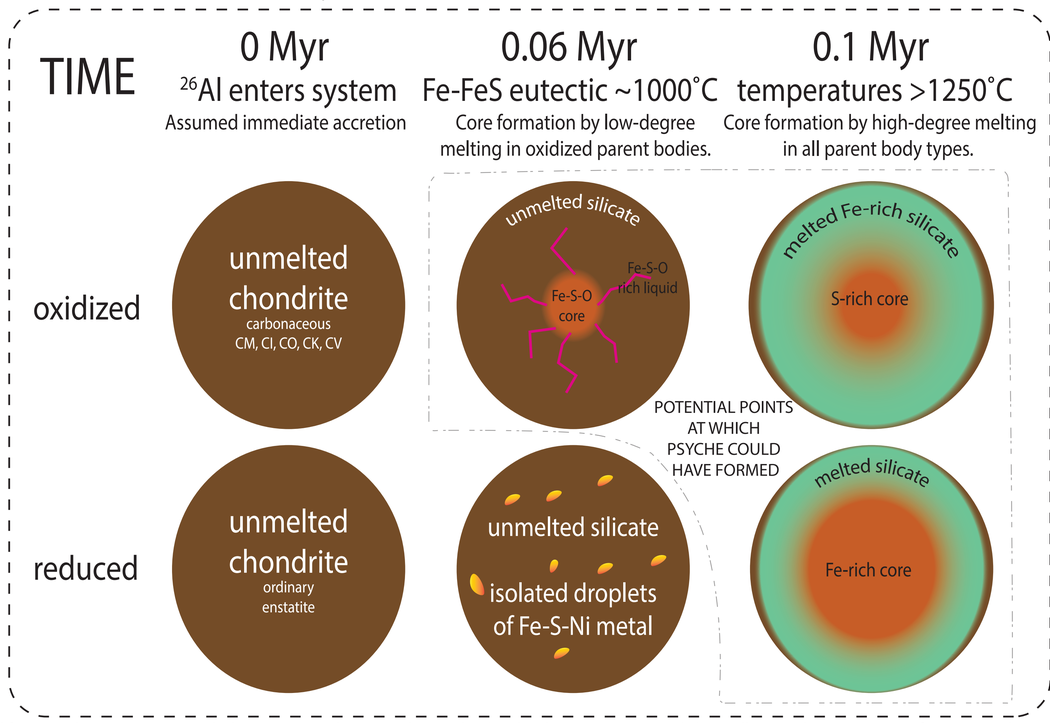

Figure 2




Our model predicts that an oxidized planetesimal would form a small and sulfur-rich core, while a reduced body would form a large and sulfur-poor core. The partition coefficient of sulfur ($D_S$) decreases linearly with increasing $\log C_S$, meaning that sulfur partitions into reduced bodies more than oxidized bodies (Fig. 1A). Reduced bodies will form larger cores than oxidized bodies (1B), and oxidized cores will have more sulfur-rich cores than reduced bodies due to the lack of free metallic iron and nickel (1C). We find that $fO_2$ affects the mineralogy of cores (Fig. 2). Our data overlaps with experimental work that predicts asteroidal core compositions [13] and Fe and Ni data for IIAB, IID and IVA iron meteorites. Iron, nickel and either modeled or measured sulfur data are from [4, 10, 13-18].

## Conclusions

1. Sulfur partitions more into a reduced parent body's core than oxidized parent body's core.
2. Oxidized parent bodies form small, sulfur-rich cores while reduced parent bodies form larger, sulfur-poorer cores [8].
3. All chondritic compositions make cores with >9 wt.% sulfur, which will cause a sulfide-rich immiscible liquid to form [9].
4. If Psyche is sulfur-rich, it could have formed before or after its parent body's silicate components totally melted (see top row below) [6].
5. If Psyche is sulfur-poor, it would have formed from a reduced body after the planetesimal totally melted (see bottom row below).

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