Constraints on the lunar core composition and thermal state from geophysical data and thermodynamic properties of liquid iron-sulfur alloys.

A. Rivoldini, M-H. Deproost, T. Van Hoolst
Observatoire Royal de Belgique

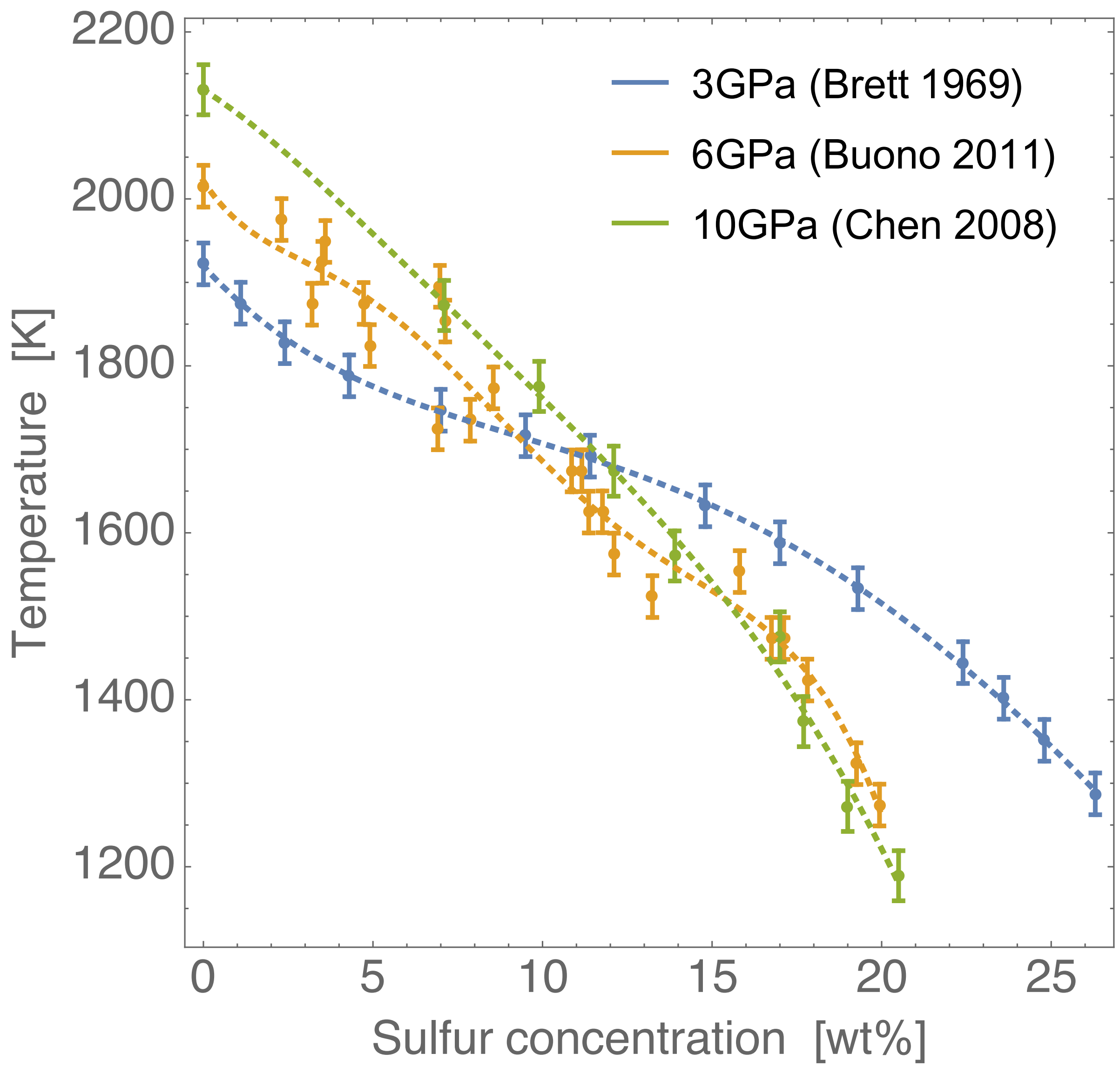
precise thermodynamic and consistent knowledge about the core required for:

- the interpretation of GRAIL results and (re)analysis of Apollo and future seismic data
- understand the thermal evolution of the core and its capacity to generate a magnetic field

⇒ thermodynamic model should agree with measured melting

data **and** elastic properties of core materials

Iron-rich liquidus

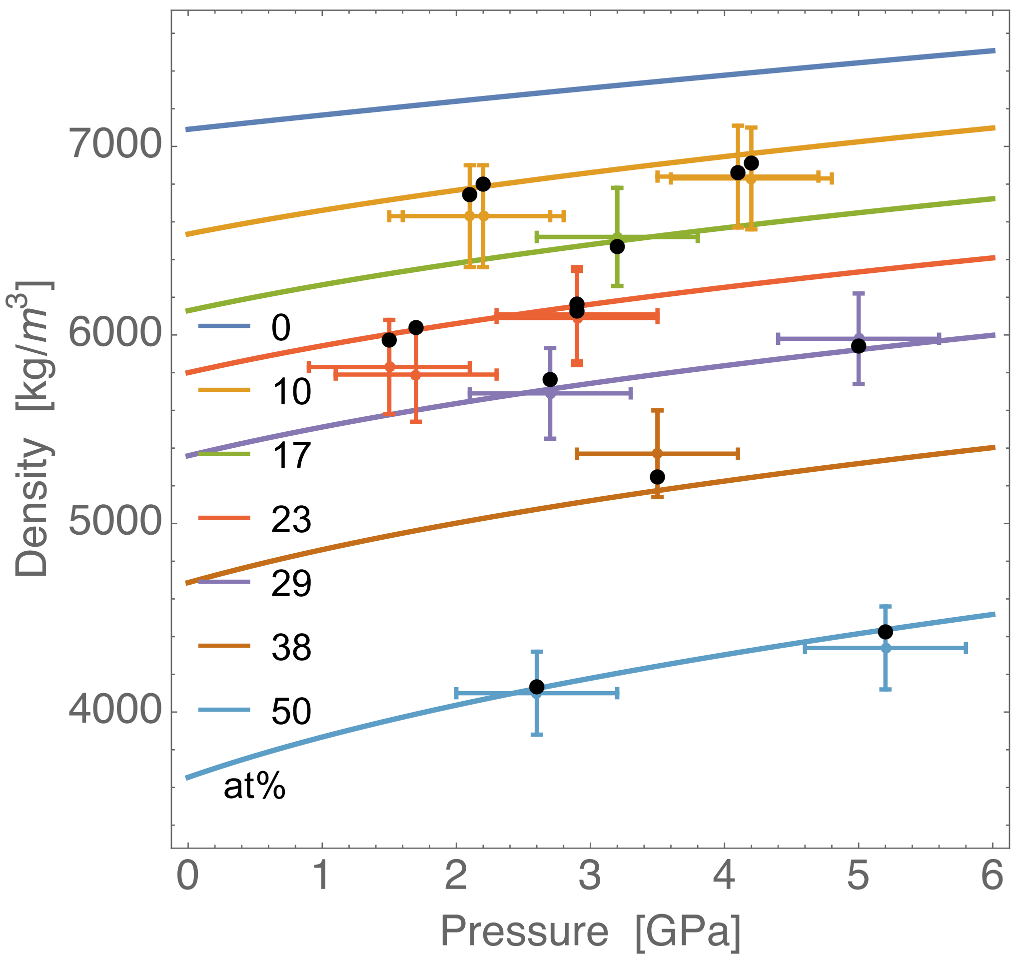


- highly non-ideal
- can be described with an asymmetric Margules model that has interaction parameters linear in p and T (Buono & Walker 2011)

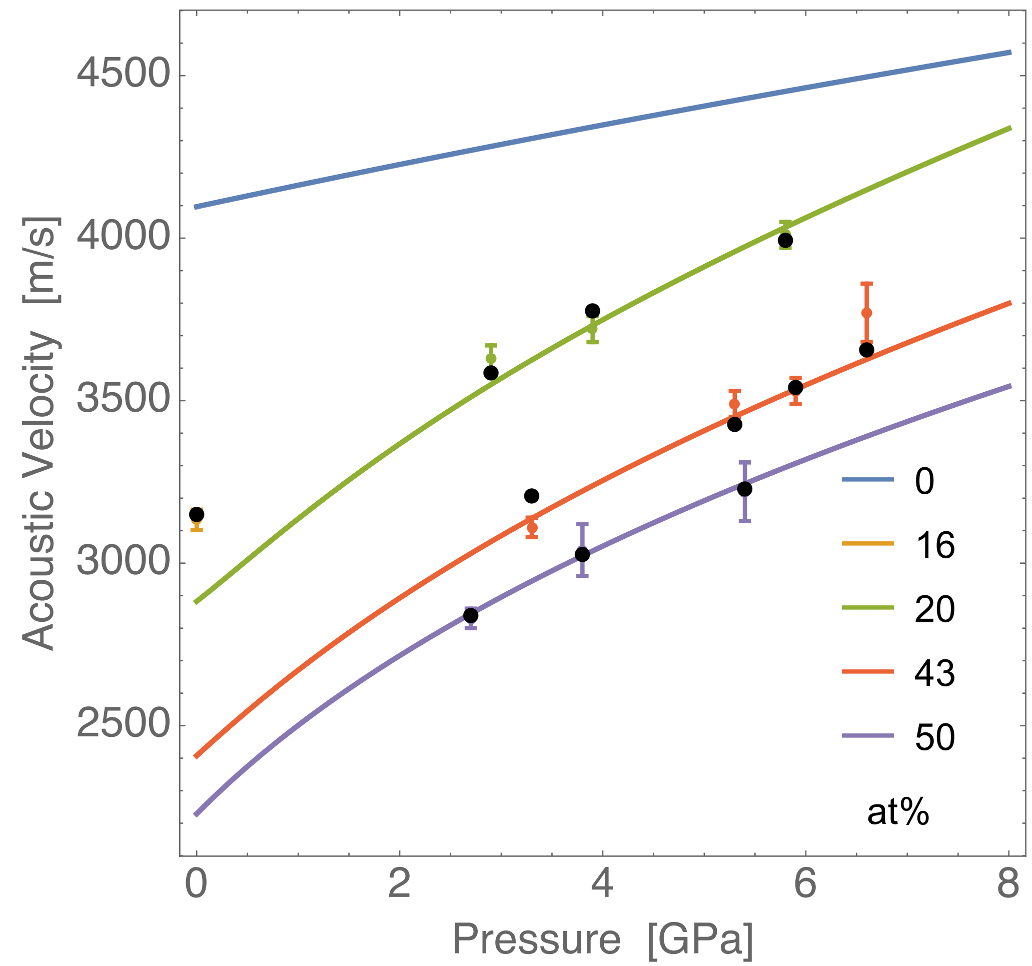
$$
\begin{aligned}
G^l(x,p,T) =& (1-x)\,G^l_{\mathrm{Fe}}(p,T) + x\,G^l_{\mathrm{FeS}}(p,T) + \\
& (1-x)\,R\,T\ln(1-x) + x\,R\,T\ln(x) + \\
& x(1-x)\left[x\,W_{\mathrm{Fe}}(p,T) + (1-x)\,W_{\mathrm{FeS}}(p,T)\right]
\end{aligned}
$$

Elastic properties

X-Ray absorption method
Morard et al. 2018



Ultrasonic pulse-echo method
Nishida et al. 2016



- Buono & Walker model induces a concentration dependent but (p,T) independent excessive mixing volume that can well summarize the high pressure density data
- **but not** the acoustic velocity data

Thermodynamic model

- end-members l-Fe (modified from Komabayashi 2014) and l-FeS
- asymmetric Margules model with pressure dependent excessive volume

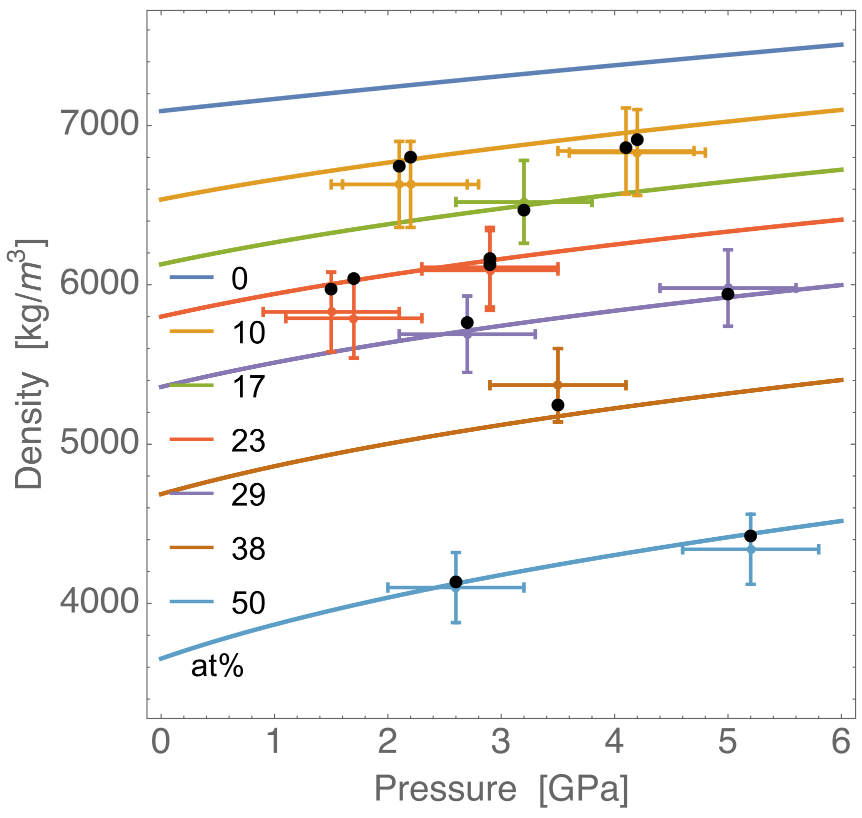
$$G^l_{ex}(x,p,T) = x(1-x)\left[x\,W_{\mathrm{Fe}}(p,T) + (1-x)\,W_{\mathrm{FeS}}(p,T)\right]$$

$$W_{\mathrm{Fe}}(p,T) = W_{\mathrm{Fe},H} - W_{\mathrm{Fe},S}T + pW_{\mathrm{Fe},V_1} + \frac{3}{2}W_{\mathrm{Fe},V_2}\left[p(\ln 2 - 1) + (1+p)\ln\left(\frac{3}{2}+p\right)\right]$$

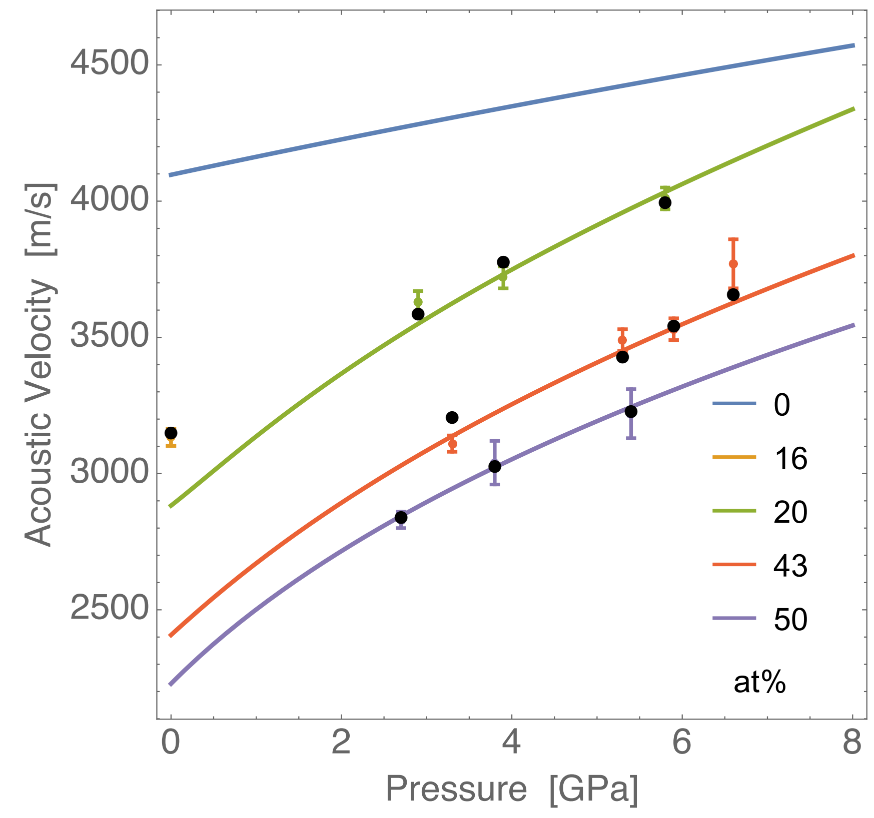
$$W_{\mathrm{FeS}}(p,T) = W_{\mathrm{FeS},H} - W_{\mathrm{FeS},S}T + pW_{\mathrm{FeS},V_1} + \frac{1}{2}p^2 W_{\mathrm{FeS},V_2}$$

- EoS parameters for FeS (4) and interaction parameters (6) are estimated from liquidus, density, and acoustic velocity data
- ambient pressure density and thermal expansivity of FeS from Kaiura & Toguri 1979

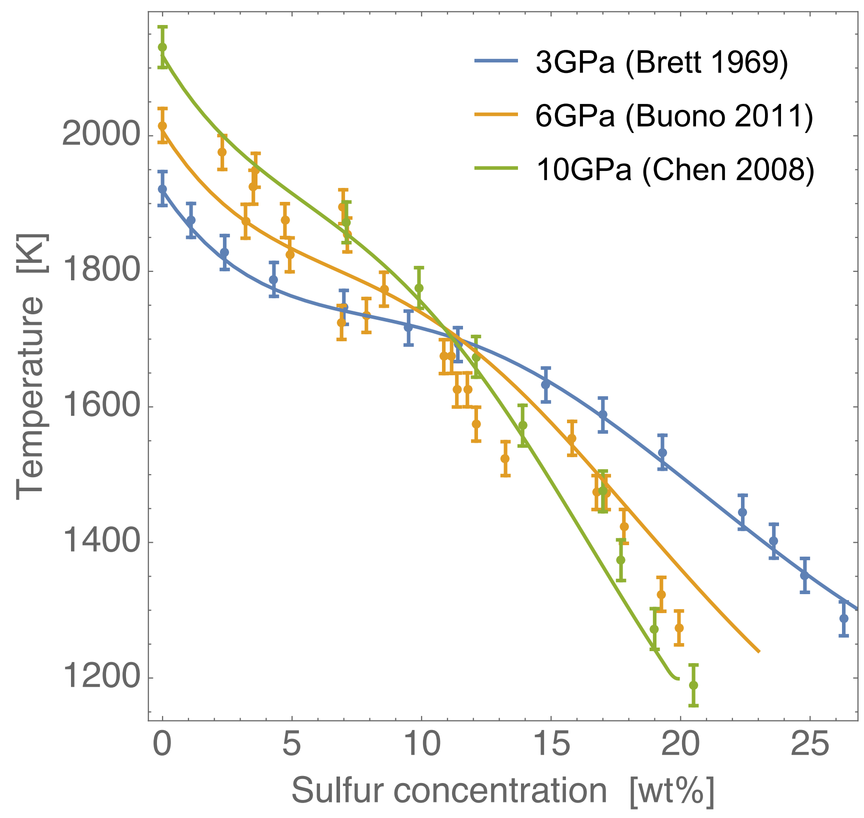
Data-Fit



Density [kg/m^3]
Pressure [GPa]
0
10
17
23
29
38
50
at%

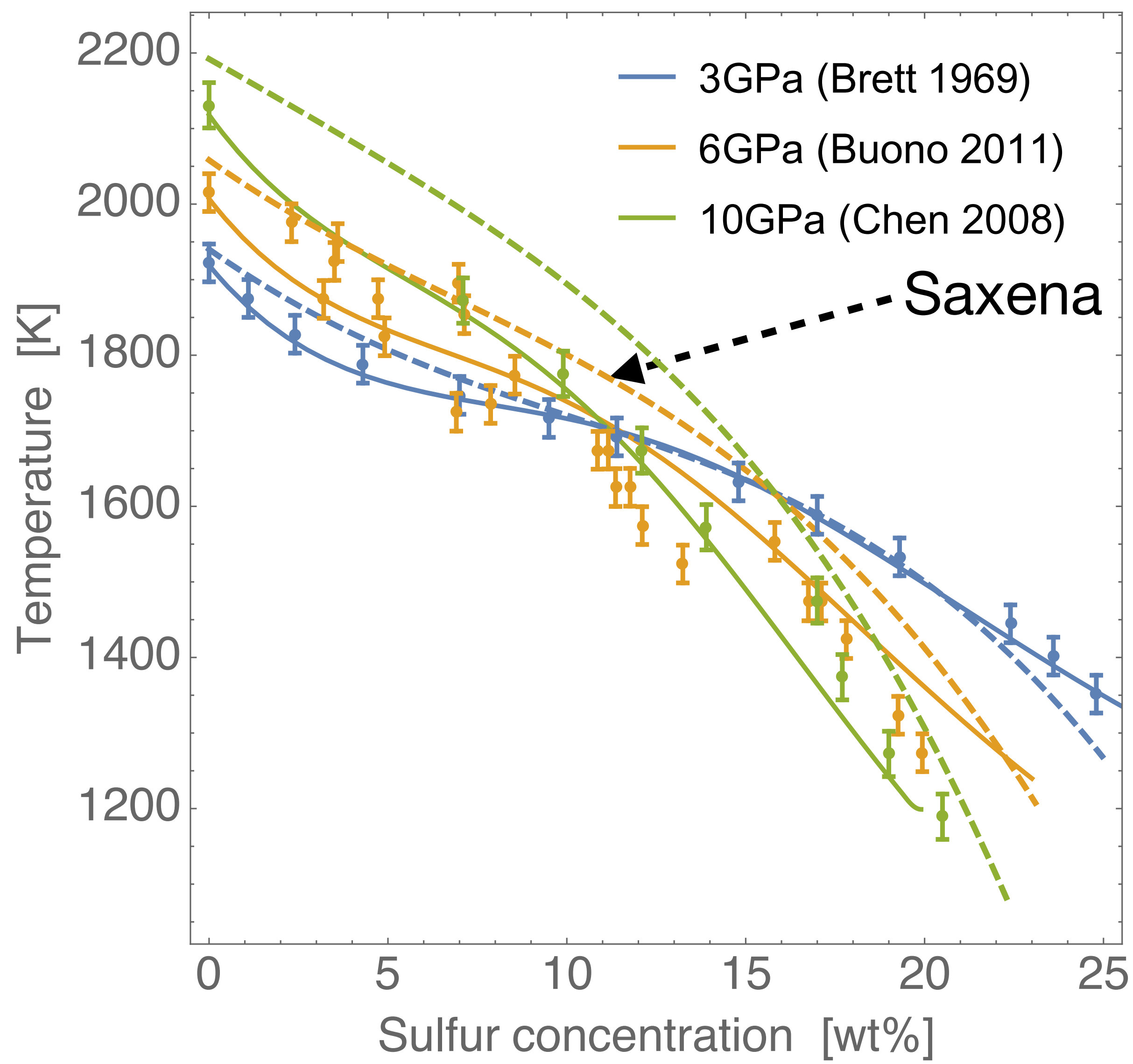


Acoustic Velocity [m/s]
Pressure [GPa]
0
16
20
43
50
at%



3GPa (Brett 1969)
6GPa (Buono 2011)
10GPa (Chen 2008)
Temperature [K]
Sulfur concentration [wt%]

Iron-rich liquidus: comparison with Saxena & Eriksson 2015

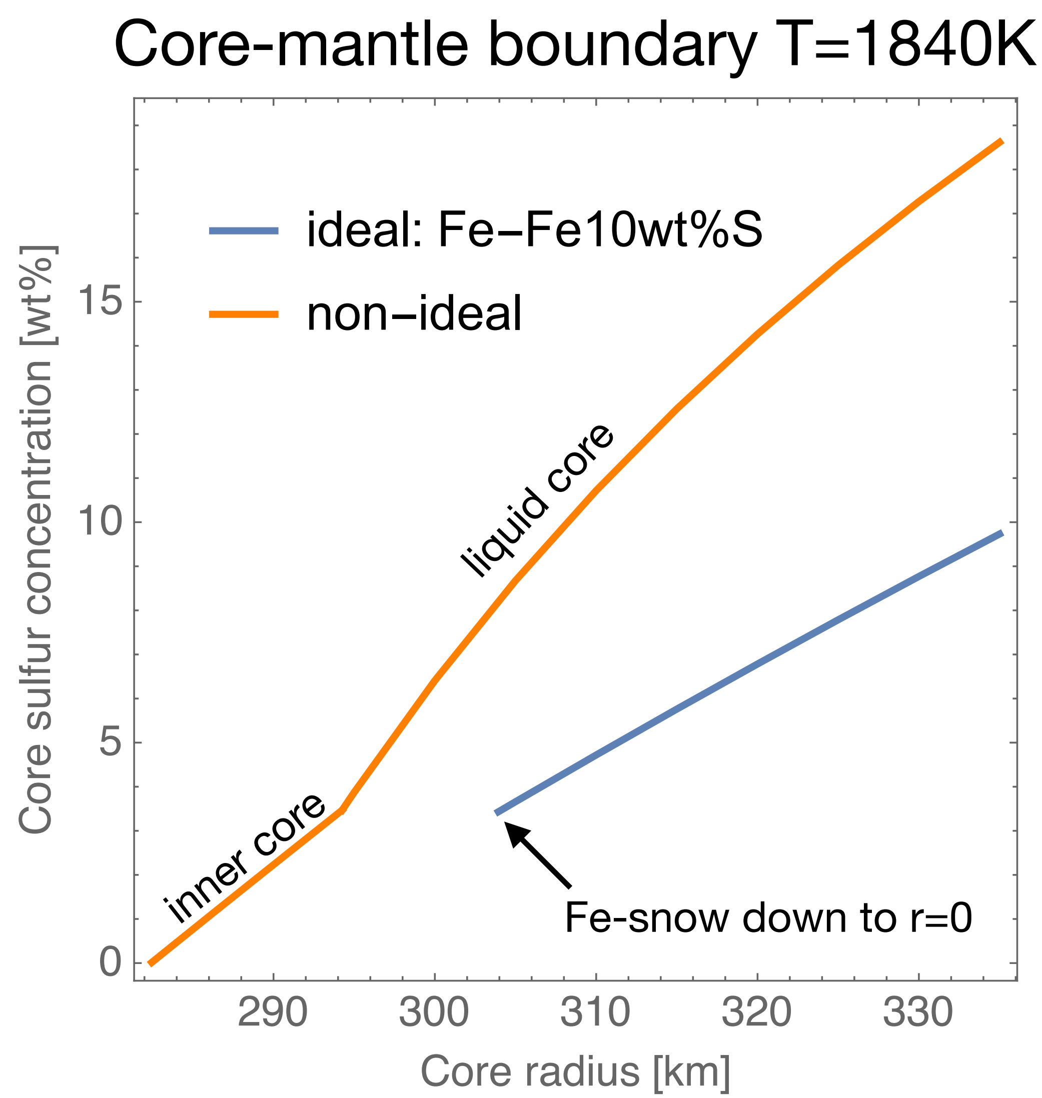


- based on modified quasi-chemical model (Waldner & Pelton 2005)
  ⇒describes precisely **whole** Fe-S phase diagram at 1bar
- extension to high pressure (~200GPa) by using high pressure eutectic data and EoS for end-members
- requires FactSage :-(((or Perple_X
- does not include above liquidus data

Moon models

- agree with the latest estimate of the average moment of inertia (MOI = 0.393112 ± 0.000012, Williams et al., 2014)
- mantle density model of Weber et al. (2011)
  upper mantle density reduced by ~0.1% to make models agree with the MOI
- core thermal evolution model based on Davies et al. (2015) and mantle evolution model based on Morschhauser et al. (2011)
- thermodynamic model of the core: this study

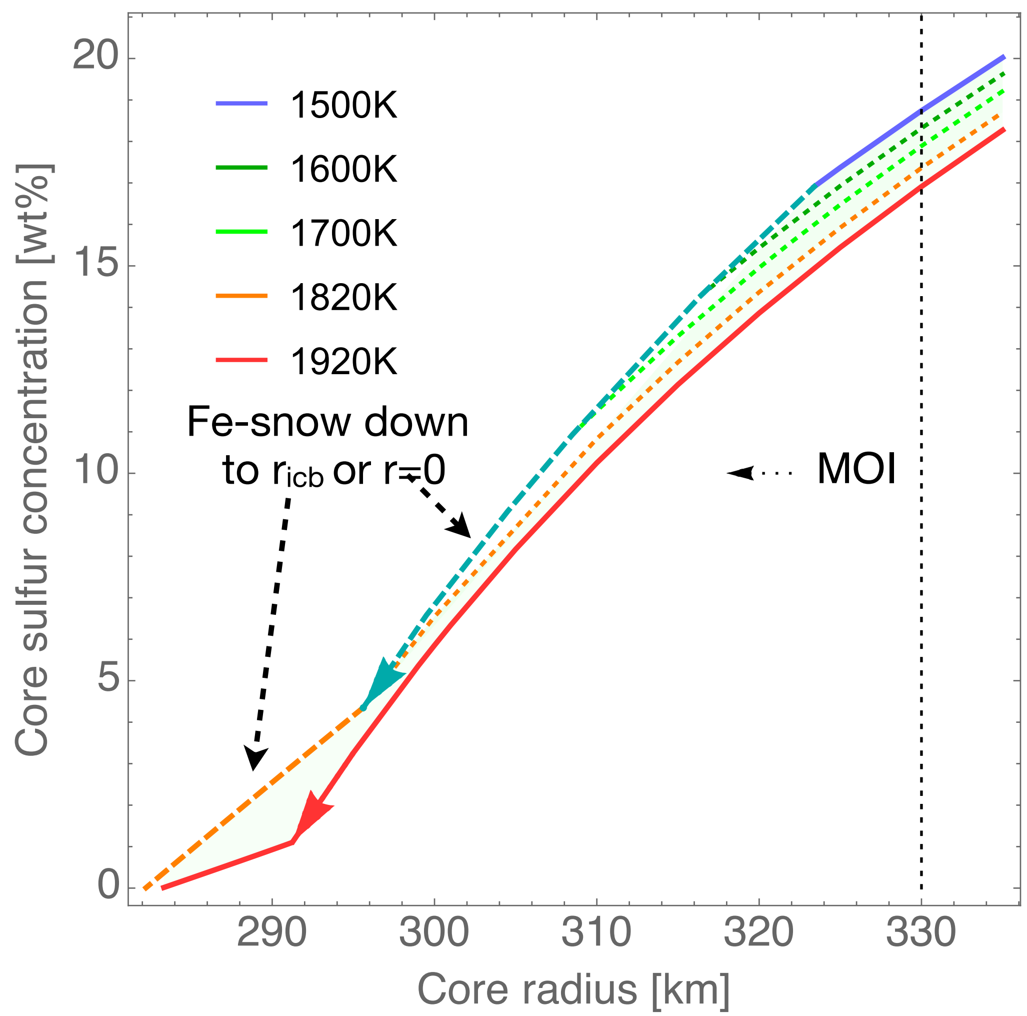
Structure functions:
Ideal versus non-ideal

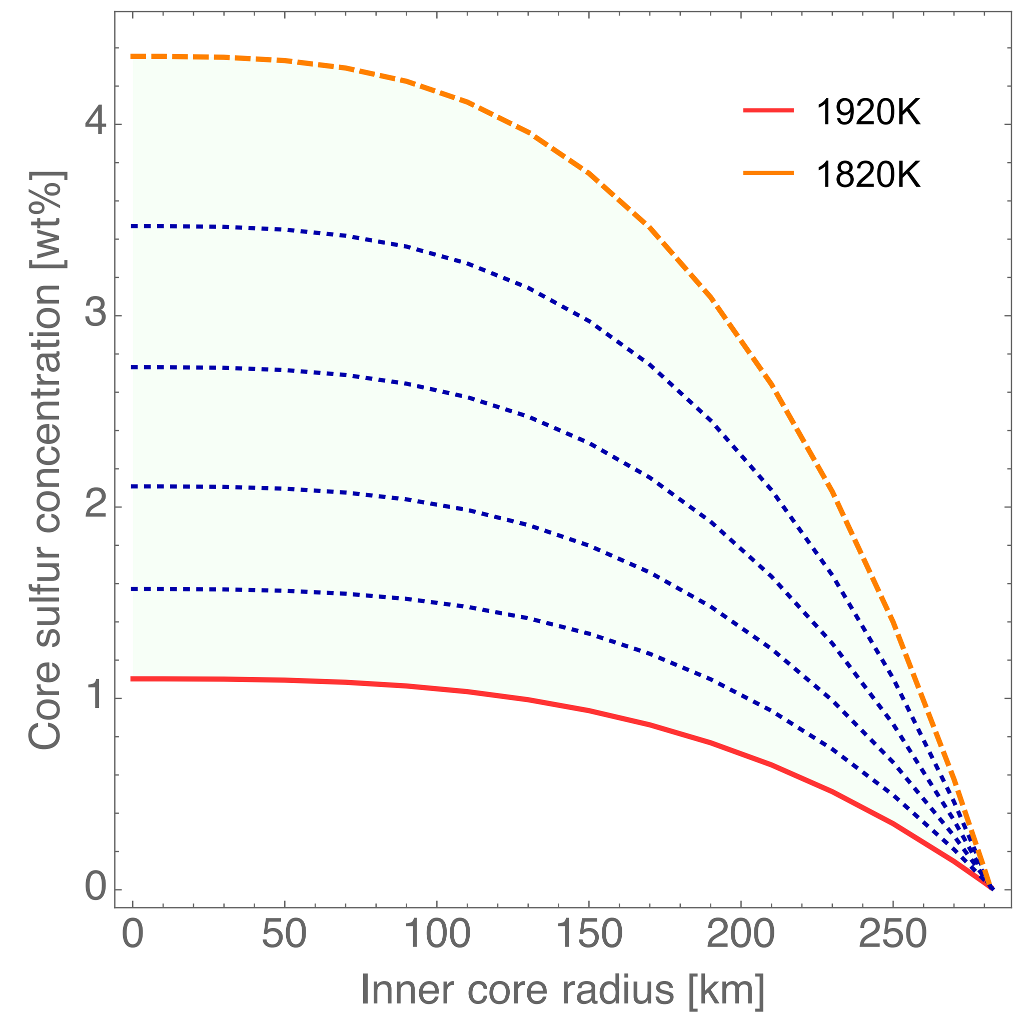


ideal model end-members:
Fe (modified from Komabayashi 2014)
Fe10wt%S (Balog et al. 2003)

- ideal model: no bottom-up inner core if $T_{cmb} \geq 1840K$
- ideal model less compressible requires less sulfur than non-ideal model for same average core density
- non-measurable effect on MOI-core radius relation and tidal Love number k_2-core radius relation

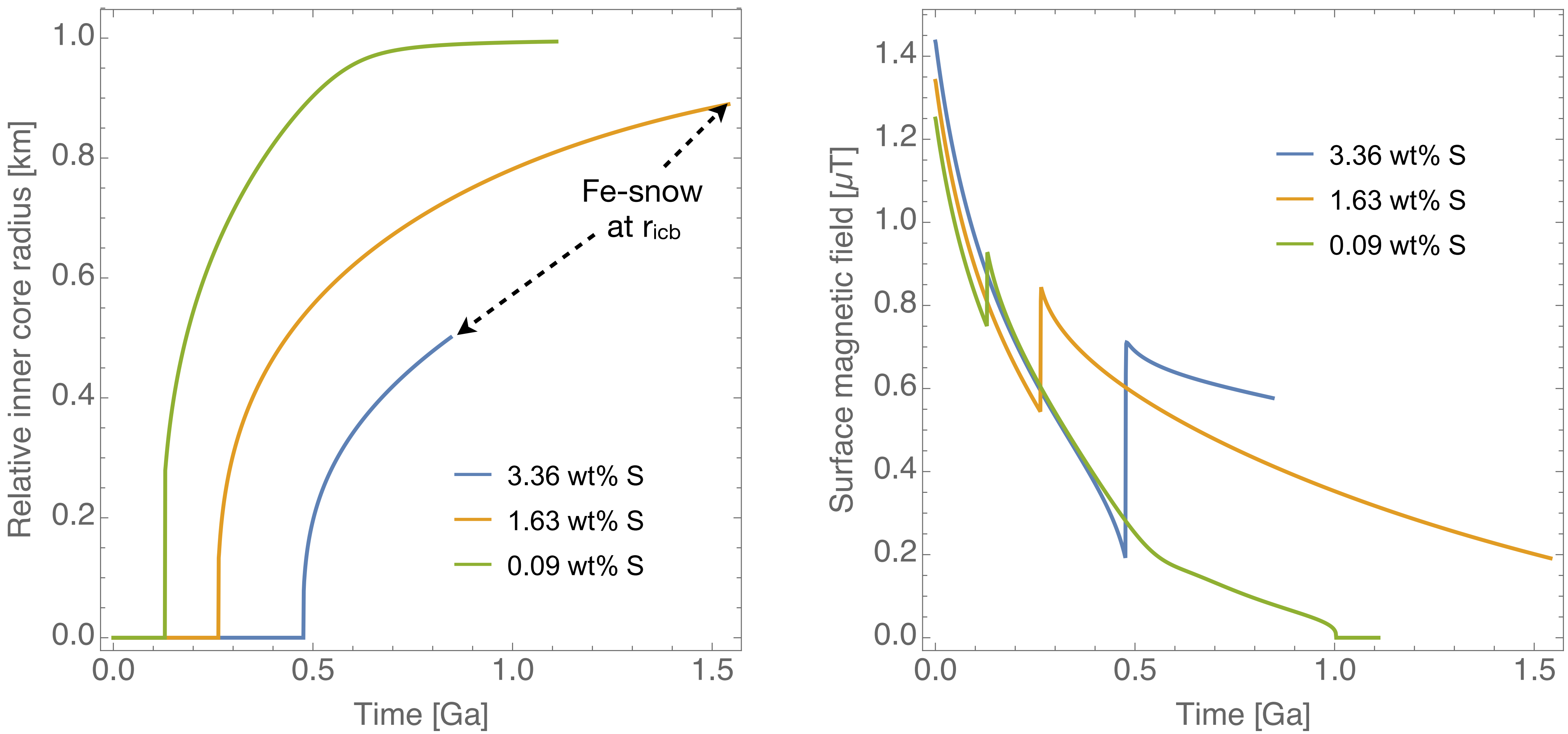
Structure functions





- to agree with MOI $T_{cmb} \gtrsim 1410$K (~19wt%S) and $r_{cmb} \lesssim 330$km
- inner core possible if $r_{cmb} \lesssim 280$km
- to avoid lower mantle melting $T_{cmb} \lesssim 1920$K (Hirschmann et al. 2012)

Thermal evolution with bottom-up inner core formation



- all required thermodynamic quantities for core thermal evolution are computed form core model of this study (density, heat capacity, latent heat of crystallization, thermal- and chemical expansivity)
- main power and entropy source is latent heat
- early dynamo possible with surface magnetic field in agreement with lunar magnetic records (≳1μT) (Garrick-Bethell et al., 2009)

Conclusions

- melting data and new elastic data about Fe-S alloys can be described with a non-ideal mixing model that has a pressure dependent excess volume

- to agree with the MOI at 1σ the core-mantle boundary temperature cannot be below ~1410K and to avoid lower mantle melting it has to be below ~1910K

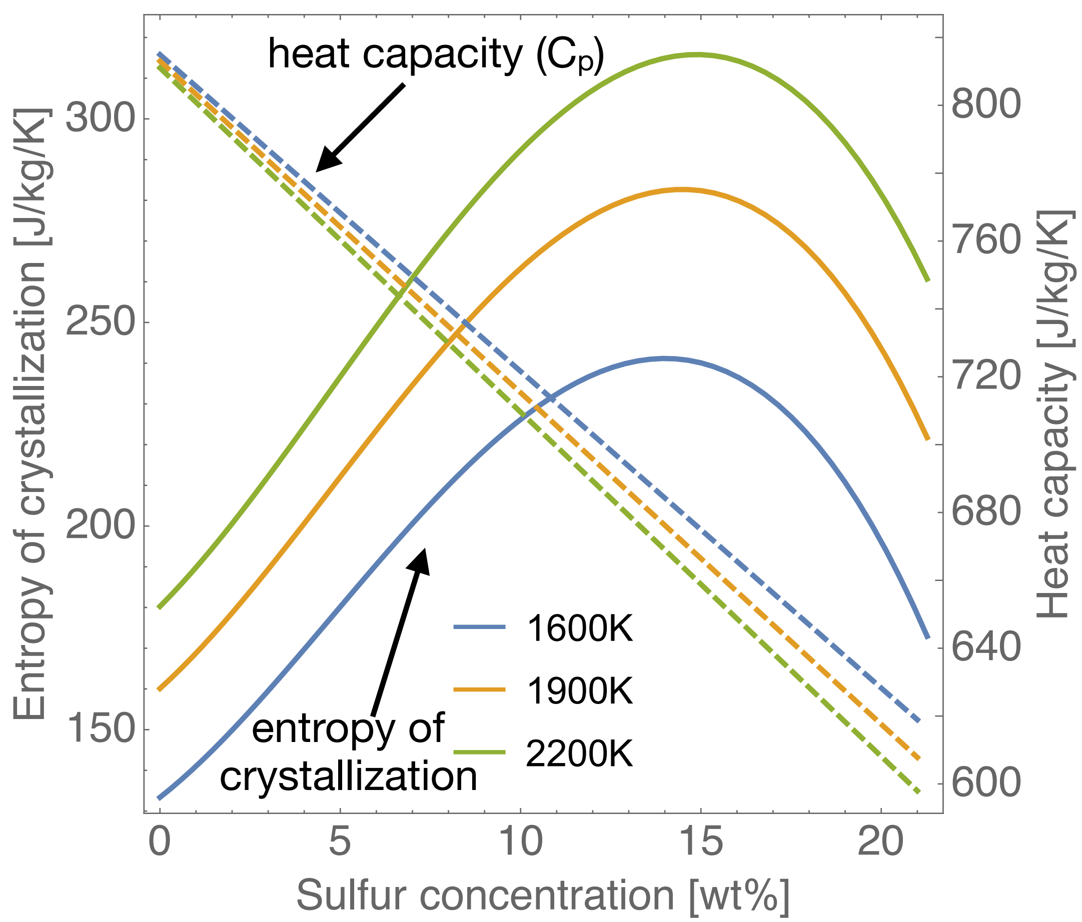
- models with an inner core and without a whole snowing liquid core cannot be much colder than ~1820K and those models have less than ~4.5wt% of sulfur

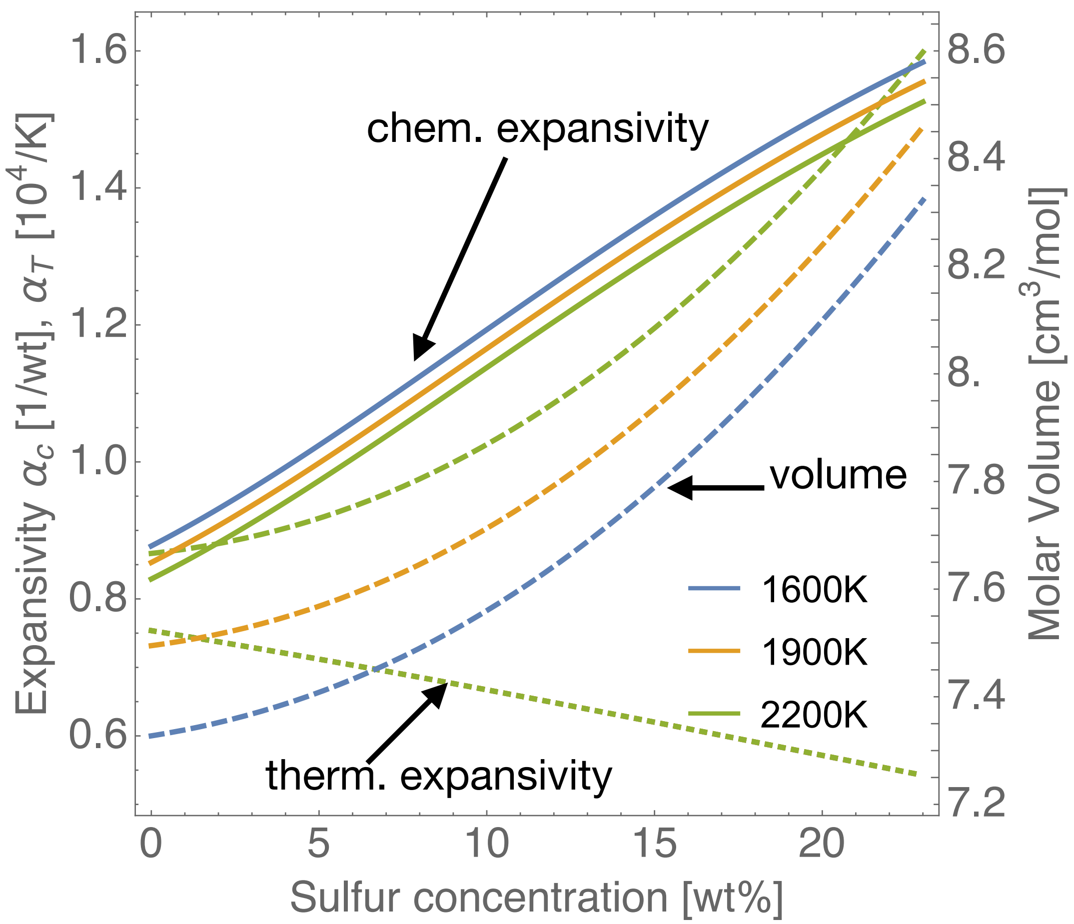
- models without an inner core having a marginal dynamo until about 3.56Gyr ago require core-mantle boundary temperatures significantly above the mantle solidus (≳2500K)

  ⇒ models without an inner core cannot generate a dynamo in agreement with observations

- models with an inner core can have an early dynamo, a core-mantle boundary temperature below the mantle solidus after ~400Ma, and an early surface magnetic field in agreement with lunar magnetic records (≳1μT) (Garrick-Bethell et al., 2009)

Thermodynamic quantities





Thermal evolution