



	Experiment title: Thermal equation of state and phase diagram of SiC under extreme conditions: implications for the interiors of C-rich planets	Experiment number: HC 2481
Beamline: ID 27	Date of experiment: from: 06/06/2016 to: 12/06/2016	Date of report: 11/09/2017
Shifts: 15	Local contact(s): Mohamed Mezouar	<i>Received at ESRF:</i>
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Report:

The present work is part of the PhD thesis work of Francesca Miozzi, hired in July 2016 on the ERC grant PlanetDIVE, (PI: G. Fiquet; co-PI: G. Morard). A scientific paper is actually in progress and should be submitted before January 2018.

According to condensation models (Bond, Brien, and Lauretta 2010), a key variable determining the chemical makeup of planets is the carbon-to oxygen ratio of the disk. In stellar nebulae with carbon–oxygen ratios in excess of 0.8, condensation models propose that solid bodies consist primarily of silicon carbide and carbon, leading to the formation of solid planets consisting of silicon, carbon, and possibly iron with minimal oxygen (Bond, Brien, and Lauretta 2010). In such planets, diamond layers could for instance have huge consequences in terms of mantle dynamic as diamond possesses very different thermal conductivity properties than silicates. Recent work on carbon-based planets has been particularly motivated by the detection of planets in the 55 Cancri system, whose C/O ratio is particularly high. In particular, the planet 55 Cancri e, whose mass–radius relationship suggests that it may be insufficiently dense to have a silicate composition (Demory et al. 2012) has been modeled as consisting of layers of carbon, SiC, and iron (Madhusudhan, Lee, and Mousis 2012).

In the present project, we decided to study the phase diagram and the EoS of SiC compound. At the time of the experiment, only one paper was dealing with a potential phase transition occurring in megabar conditions observed in static compression at room

temperature (Yoshida et al. 1993). But in 2017, already two papers dealing with SiC EoS (Nisar et al. 2017) and SiC phase transition (Daviau and Lee 2017) under high pressure have been published. The present topic is therefore quite hot in the high pressure mineral physics community.

Starting material consisted in a Plasma Vapor Deposition film of Si and C mixture, originally sputtered on glass slide, with a thickness of $\sim 5\mu\text{m}$ (DEPHIS company). Such sample was able to absorb the YAG laser. Sample was scratched from this surface and loaded between two disks of KCl, used as pressure medium and pressure calibration (Dewaele et al. 2012). The small thermal expansion of KCl allows us to use it as pressure calibrator, assuming an average temperature between diamond at 300 K and the hotspot (Campbell et al. 2009). Diamonds with different culet sizes were used in order to span the pressure range from 25 to 200 GPa and temperature up to 3500 K.

XRD experiments were performed using the laser heating experimental set up available on the beamline ID27. The stability of the laser and the X-ray alignment allowed us to achieve isothermal compression, fixing the temperature and activating the gas membrane of the Diamond Anvil Cell (DAC) in order to define with a great accuracy the phase boundary between the two polymorphs of SiC.

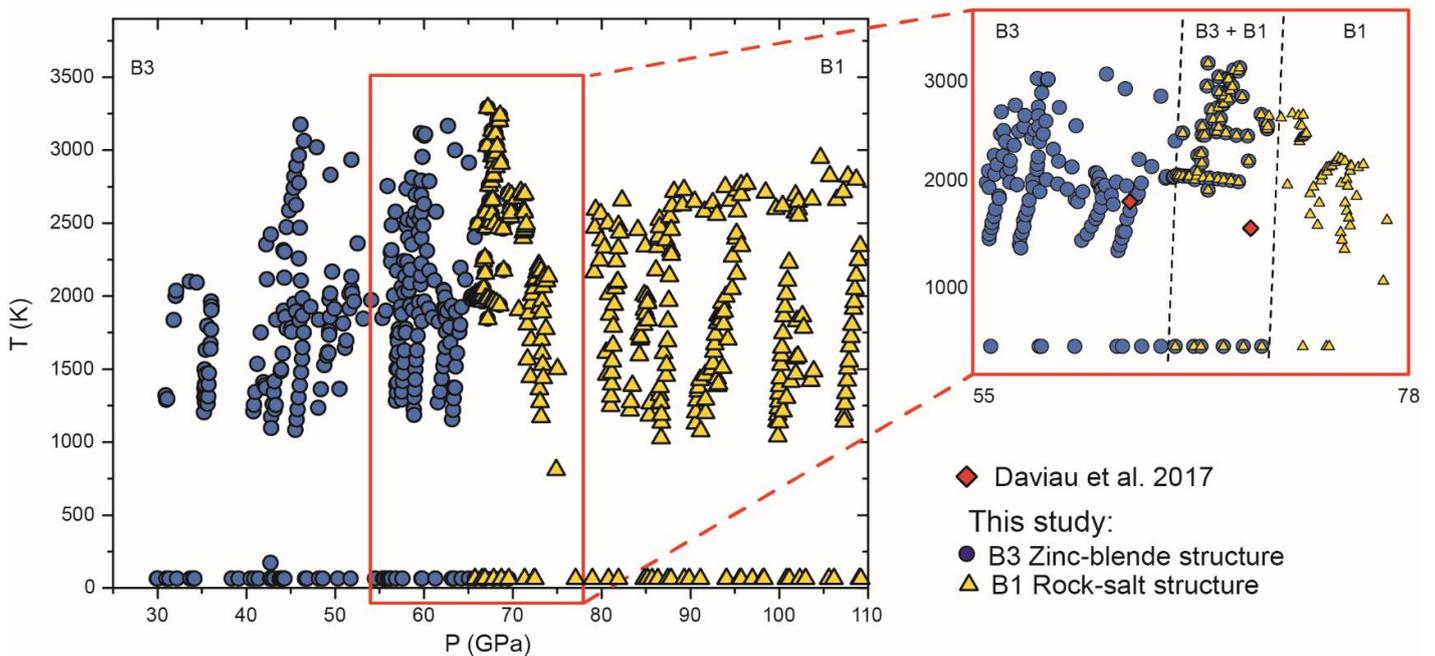


Figure 1: Phase boundary between B3 and B1 structure of SiC.

Our study allows us to establish with accuracy the Clapeyron slope of the high pressure transition between low pressure B3 Zinc-blende structure and high pressure B1 rock-salt structure, and complement the poorly constrained (only two points) previous experiment (Daviau and Lee 2017). In addition this phase transition is accompanied by a volume collapse of almost 20%. The measurement of this phase boundary is quite important regarding the dynamic of SiC-rich exoplanets.

In addition to the phase determination, the pressure-volume data set has been fitted using a Mie-Gruneisen Deby thermal equation of state. The large pressure-temperature range investigated for the B1 structure give us confidence for the quality of the parametrization. The thermal EoS was obtained using the EoSFit software.

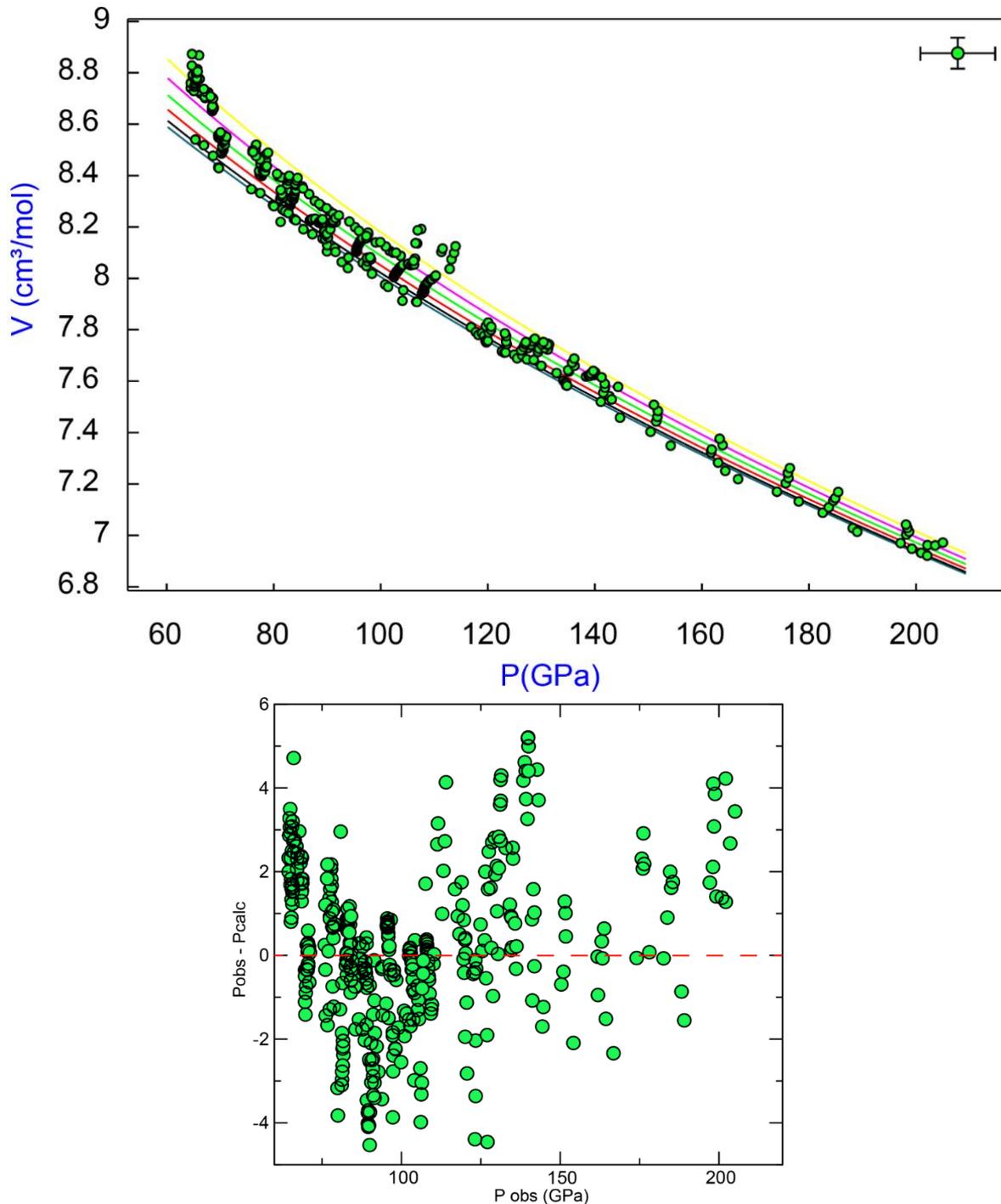


Figure 2 : Top : Volume of the B1 structure as a function of pressure and temperature fitted using EoSFit software. Different isotherms are indicated (300K, then from 1000 K to 3000 K every 500 K). Bottom : Difference between observed pressure and pressure calculated using the fit for all the data points.

Finally, the starting composition used in the present work were not SiC stoichiometric, but either Si+SiC or SiC+C. In the whole pressure range investigated, it should be noticed that no intermediate compound was found to be stable, contrary to theoretical works predicting a SiC₂ compound around 25 GPa (Andrew, Braun, and Chetty 2012). On the Si-rich side, melting was tracked around 2000 K in the 50-70 GPa pressure range, indicating a potential eutectic melting on this side of the phase diagram.

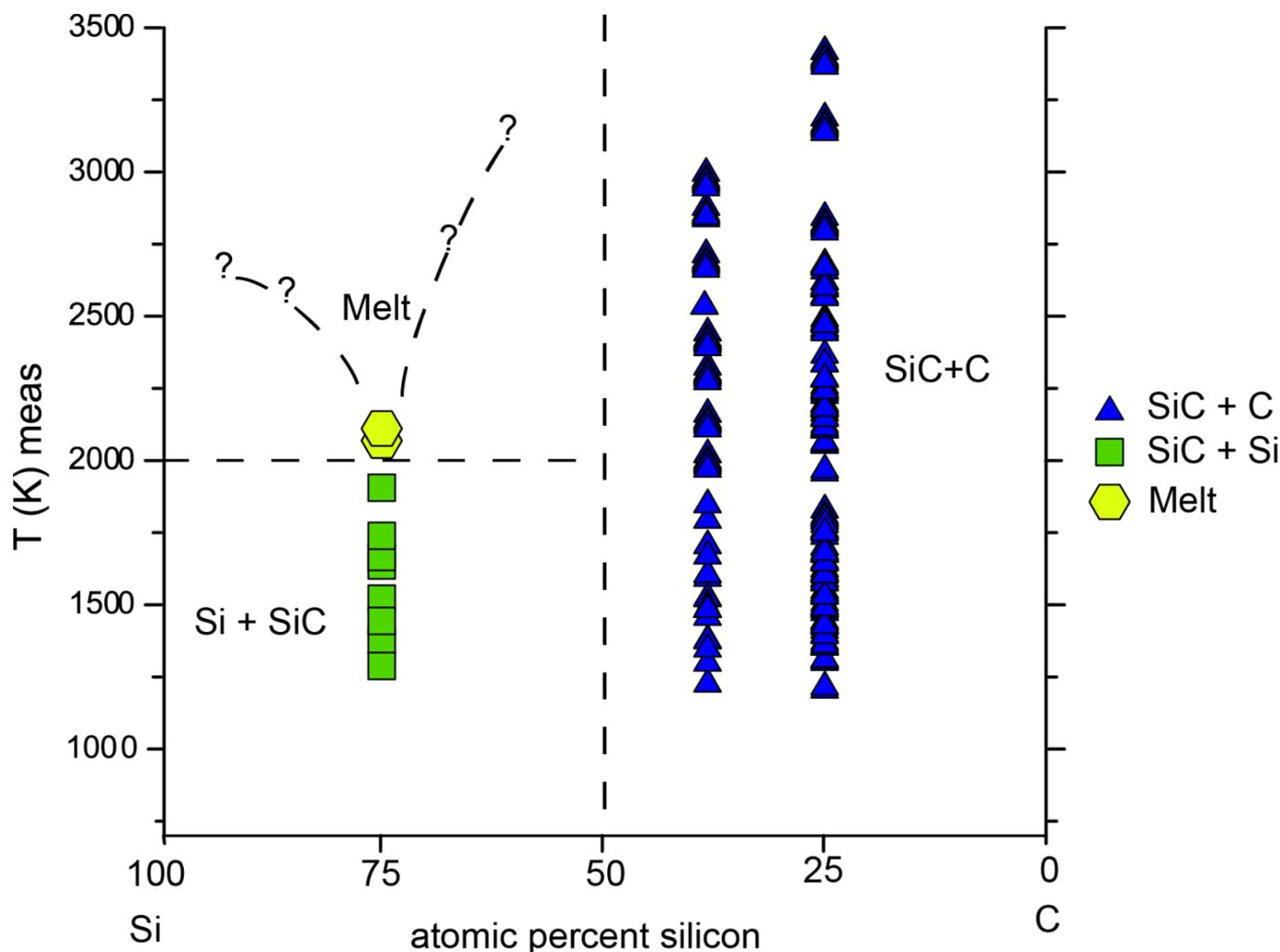


Figure 3: Si-C binary phase diagram at pressure conditions between 50 and 80 GPa.

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