MAR16-2015-000845

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Study of the Warm Dense Matter with XANES spectroscopy - Applications to planetary interiors

ADRIEN DENOEUD, CEA

With the recent discovery of many exoplanets, modelling the interior of these celestial bodies is becoming a fascinating scientific challenge. In this context, it is crucial to accurately know the equations of state and the macroscopic and microscopic physical properties of their constituent materials in the Warm Dense Matter regime (WDM). Moreover, planetary models rely almost exclusively on physical properties obtained using first principles simulations based on density functional theory (DFT) predictions. It is thus of paramount importance to validate the basic underlying mechanisms occurring for key planetary constituents (metallization, dissociation, structural modifications, phase transitions, etc....) as pressure and temperature both increase[1,2].

In this work, we were interested in two materials that can be mainly found in the Earth-like planets: silica, or SiO2, as a model compound of the silicates that constitute the major part of their mantles, and iron, which is found in abundance in their cores. These two materials were compressed and brought to the WDM regime by using strong shock created by laser pulses during various experiments performed on the LULI2000 (Palaiseau, France) and the JLF (Livermore, US) laser facilities and on the LCLS XFEL (Stanford, US). In order to penetrate this dense matter and to have access to its both ionic and electronic structures, we have probed silica and iron with time-resolved X-ray Absorption Near Edge Structure (XANES)[3]. In parallel with these experiments, we performed quantum molecular dynamics simulations based on DFT at conditions representative of the region investigated experimentally so as to extract the interesting physical processes and comprehend the limits of the implemented models[4]. In particular, these works allowed us to highlight the metallization processes of silica in temperature[5] and the structural changes of its liquid in density, as well as to more constrain the melting curve of iron at very high pressures.

[1]K. Umemoto et al., Science 311, 983 (2006)
[2]D. Hicks et al., Phys. Rev. Lett, 97, 025502 (2006)
[3]A. Benuzzi-Mounaix et al., Phys. Rev. Lett, 107, 165006 (2011)
[4]V. Recoules et al., Phys. Rev. B, 80, 064110 (2009)
[5]A. Denoeud et al., Phys. Rev. Lett, 113, 116404 (2014)