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ID-28:18	G. Garbarino (ID-27)	
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Names and affiliations of applicants (* indicates experimentalists):		
• *D. Antonangeli, *F. Decremps, *E. Edmund, *G. Fiquet, *G. Morard, Sorbonne		

Université, CNRS, IMPMC, Paris, France.
*Y. Fei, Geophysical Laboratory, Carnegie Institution, Washington, USA.

Report:

We performed inelastic x-ray scattering and x-ray diffraction measurements to determine sound velocity and density of a polycrystalline Fe-Si alloy with 9 wt.% Si in the hcp phase at 42 and 59 GPa, complementing previously obtained data set (experimental report ES-222).

Pressures were generated by symmetric type MAO DAC, equipped with 150/300 μ m bevelled anvils and Re gaskets. Pressure was measured off line by collecting Raman spectra at the tip of the diamonds, and crosscheck after collection of sample diffraction by using previously established equation of state.

IXS measurements have been performed on polycrystalline samples compressed in a diamond anvil cell (DAC) using the Si(9,9,9) instrument configuration. The Si(9,9,9) configuration has been proven to enhance the contrast between sample and diamonds phonons with respect to data obtained using the Si(8,8,8) configurations as typically done for powders in DAC (the widths of diamond phonons are defined by the energy resolution of the spectrometer), still providing enough flux to collect good-quality data in reasonable amount of time (~500-600 s per point). Spectra have been collected in transmission geometry, with the x-ray beam impinging on the sample through the diamonds, along the main compression axis of the cell, and hence probing exchange momenta q perpendicular to the cell-axis. The x-ray beam was focused at sample position to 30x70 µm² (horizontal x vertical, FWHM) by optics in Kirkpatrick-Baez configuration. Momentum resolution was set to 0.28 and 0.84 nm⁻¹ in the horizontal and vertical plane. A vacuum chamber was used to minimize the quasi-elastic scattering contribution from air. At each investigated pressure point, we mapped the aggregate longitudinal acoustic phonon dispersion throughout the entire first Brillouin zone collecting 9 spectra in the 3-12.5 nm⁻¹ range. The energy positions of the phonons were extracted by fitting a set of Lorentzian functions convolved with the experimental resolution function to the IXS spectra, utilizing a standard χ^2 minimization routine. We then derived the aggregate compressional sound velocity V_P from a sinus fit to the phonon dispersion, with error bars between ± 2 and $\pm 4\%$. Combining the measured V_P with bulk modulus K from the equation of state (the difference between isothermal and adiabatic bulk modulus at 300K is negligible), we also derived $V_{\rm S}$, with uncertainties, obtained by propagating uncertainties on $V_{\rm P}$ and on K (the contribution from uncertainties on density was ob-served to be negligible), between ± 8 and $\pm 10\%$.

At each investigated pressure point we collected 2D diffraction patterns on ID27. Tacking advantage of the $3x3 \ \mu m^2$ beam, we collected data over the entire sample surface, monitoring pressure gradients. Collected diffraction pattern have been analyzed to determine sample's texture as well.

More details concerning the scientific results and their significance can be found in:

"Sound velocities and density measurements of solid hcp-Fe and hcp-Fe–Si (9wt.%) alloy at high pressure: Constraints on the Si abundance in the Earth's inner core", D. Antonangeli et al., Earth and Planetary Science Letters 482 (2018) 446–453.