EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

	Experiment title: Sound velocities in the Fe-Si-C alloys at extreme conditions: Si and C in the core	**Experiment number**: ES-1111
Beamline: ID18 ID15b	**Date of experiment**: from: 25.11.2021 to: 30.11.2021 from: 24.11.2021 to: 27.11.2021	**Date of report**: 02.03.2022 *Received at ESRF:*
Shifts: 15 9	**Local contact(s)**: Georgios Aprilis Davide Comboni	

Names and affiliations of applicants (* indicates experimentalists):

Ilya Kupenko*, Efim Kolesnikov*, Susanne Müller*, Carmen Sanchez-Valle

Institut für Mineralogie, University of Münster, Corrensstr. 24, 48149 Münster, Germany

Report:

During the experiment, we performed nuclear inelastic scattering (NIS) measurements upon compression of iron alloyed with silicon and carbon up to 143 GPa and laser heating at thousands of degrees. The NIS experiments were conducted using the facilities of the ID18 beamline coupled with the portable laser-heating system for diamond anvil cells. The high-pressure chambers for the experiment were prepared from Be gaskets. The alloys in the Fe-Si-C system were pre-synthesized in the University of Münster employing piston-cylinder and multianvil high-pressure apparatuses. The synthesized materials were characterized by the microprobe and diffraction analysis. Polycrystalline samples with the linear dimensions of ~10x10x10 μm^3 were loaded into the pressure chamber together with the KCl that served as a pressure transmitting medium and a thermal insulator. Panoramic diamond anvil cells specially designed for laser-heating experiments were employed for a high-pressure generation.

Data processing is currently in progress. We utilize the nuclear inelastic scattering spectra for extracting the partial phonon density of states of iron and determination of the Debye phonon average velocity (V_D). V_D is most sensitive to shear velocity (i.e. 90% of the V_D value comes from shear velocity). V_D together with density and bulk modulus, provided through the equation of state that we determined in the complementary experiment, are the necessary parameters for calculating the shear compressional velocities of the material. Figure 1A shows the energy dependence of nuclear inelastic scattering of $Fe_{0.96}Si_{0.04}C_{0.02}$ alloy at 102(1) GPa at room temperature and 1500 K. Figure 1B and 1C show corresponding reduced partial phonon density of states of iron The extrapolation of the low energy region of RDOS to zero energy is required for determination of sound velocities.

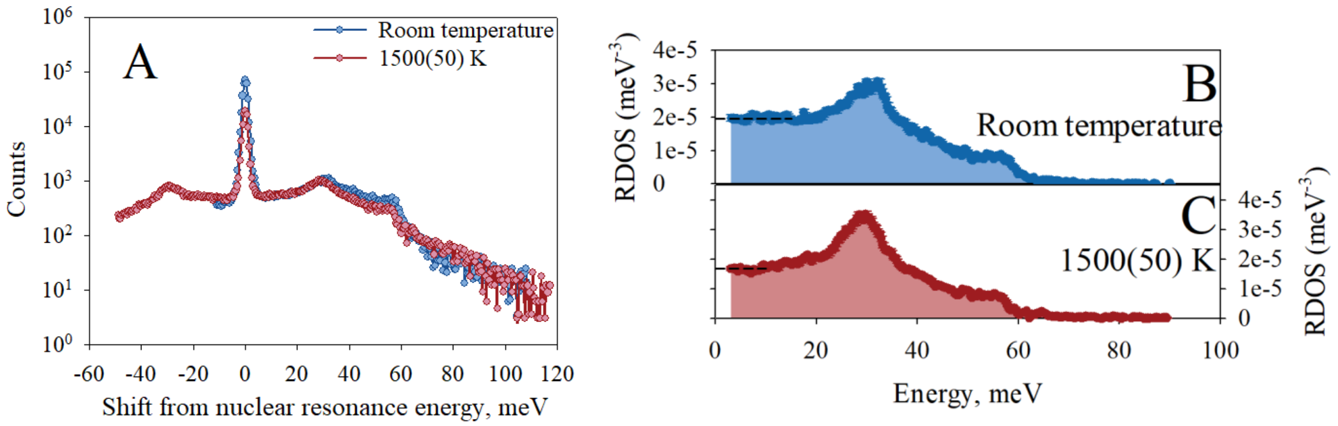

Fig.1. Energy dependence of nuclear inelastic scattering (A) and reduced partial phonon density of states (B, C) for iron for $Fe_{0.96}Si_{0.04}C_{0.02}$ alloy at 102(1) GPa at room temperature (A, B) and 1500 K (A, C). The dashed horizontal lines in (B) and C show the expected contribution of acoustic modes, that is, the Debye level.

During the diffraction experiment, we measured the pressure dependence of the unit cell volume of the $Fe_{0.96}Si_{0.04}C_{0.02}$ alloy up to 164 GPa (Fig.2). The experiment was conducted using the facilities of the ID15b beamline. The high-pressure chambers for the experiment and sample loading were prepared as described above but from Re gaskets. These data will be used to construct the P-V equation of state of the alloy. Then it will be combined with parameters for thermal parametrization of the equation of states extracted from the NIS data.

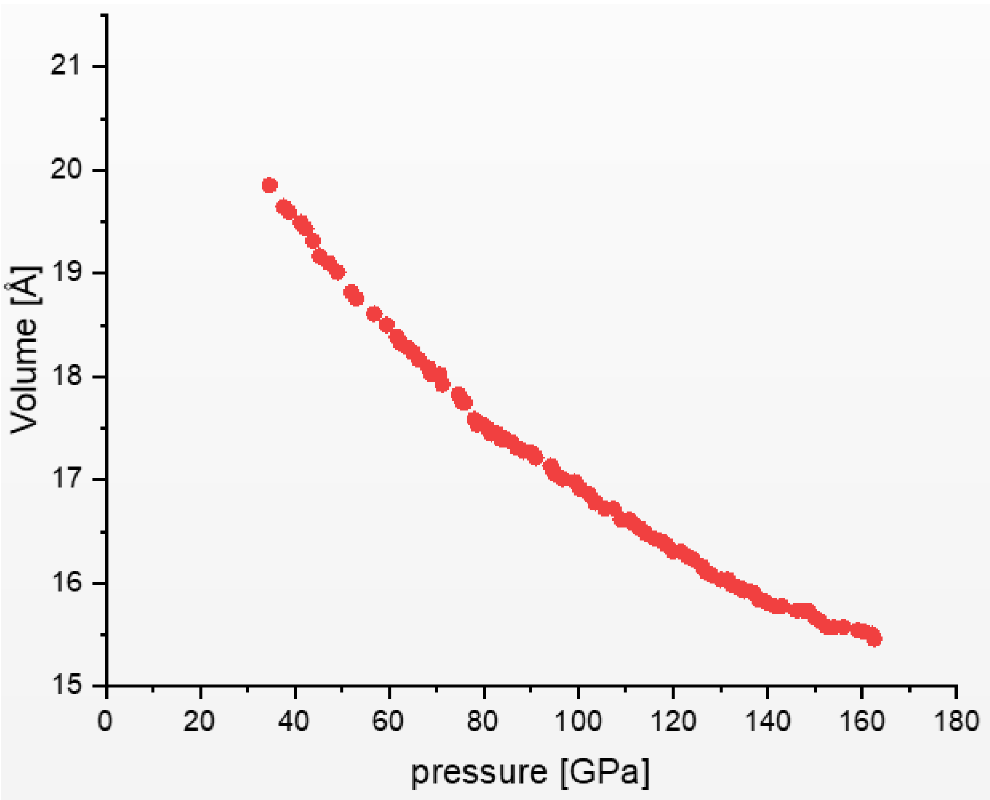

Fig.2. Pressure dependence of the unit cell volume of the $Fe_{0.96}Si_{0.04}C_{0.02}$ alloy at room temperature.