Usage Report for Fiscal Year 2018

Project Title:

Magma from the early Earth to the current Earth

Name:
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1. Background and purpose of the project, relationship of the project with other projects

The aim of the research is to clarify the history of magma in the current Earth. By using DFT and first-principles molecular dynamics, the properties of magma under extreme conditions in the Early Earth can be obtained. The simulation is expected to reveal the origin of magma in the current Earth. The high-performance parallel clusters are required to carried out first-principles calculations for amouphous, melts and liquid structures.

This project is related to the project Q18246.

2. Specific usage status of the system and calculation method

System: Hokusai bwmpc

Jobs: vnode=4, vnode-core=40, vnode-mem=60000Mi

Used: ~80% of total allocated CPU hours.

Method: meta-GGA(SCAN) + van der Waals (rVV10) functional implemented in Quantum Espresso package.

To compare with X-ray Raman Scattering (XRS) measurement, we carried out XRS simulations which is implemented in Xspectra module in Quantum Espresso package.

First, we optimized both lattice parameters and atomic coordinates of epsilon-oxygen from 10 GPa to 140 GPa. The initial structure was obtained from experimental data at 17 GPa[1]. The optimized structures then will be used for XRS calculation. We used the combination of MetaGGA(SCAN) and van der Waals functionals (rvv10) [2] with 8atoms/cell for both optimization and XRS calculation. The size of the unit cell is about 4.7*4.7*3.8 ($Å^3$).

In the XRS calculation, the dipole approximation with the consideration of core-hole effects was used to calculate the transition probability from ground state to excited states where the core electron of one of three unequivalent atoms was excited to the conduction band due to the Raman scattering. The final spectrum was the average of three spectra. We applied the PAW method which was implemented in Quantum Espresso package to reconstruct the all electron states. The effects of core-hole are indicated in Fig.1. When core-electron was excited to the conduction band, the core-hole will be partially screened by surrounding electrons. Therefore, we consider fractional core-hole. We show the spectra at 10 GPa calculated with differently fractional core-holes in comparison with experimental data [3]. The core-hole effects shift the conduction bands, especially around 10 eV, to lower energy. The intensities of the π^* and σ^* peaks suggests that 0.5 core-hole model is a good choice since the experimental intensity has been well reproduced.

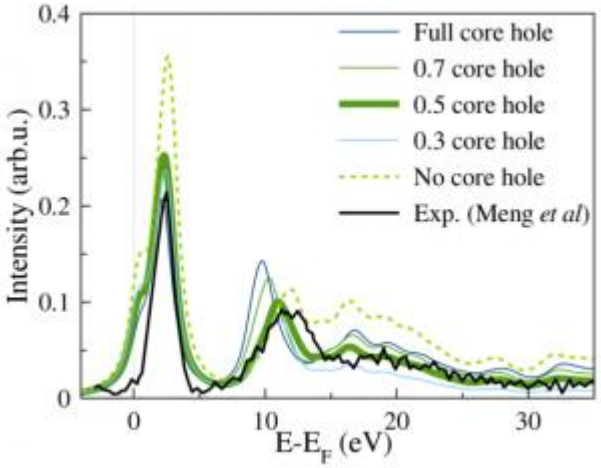

Figure 1. The effects of fractional core-hole on the XRS spectra.

3. Result

The calculated XRS are qualitatively comparable with room temperature XRS measurement at high pressure (>60 GPa). The epsilon-zeta transition can be clarified by comparing calculated XRS and measured XRS.

The spectra at < 40 GPa needs to be carefully considered in simulation.

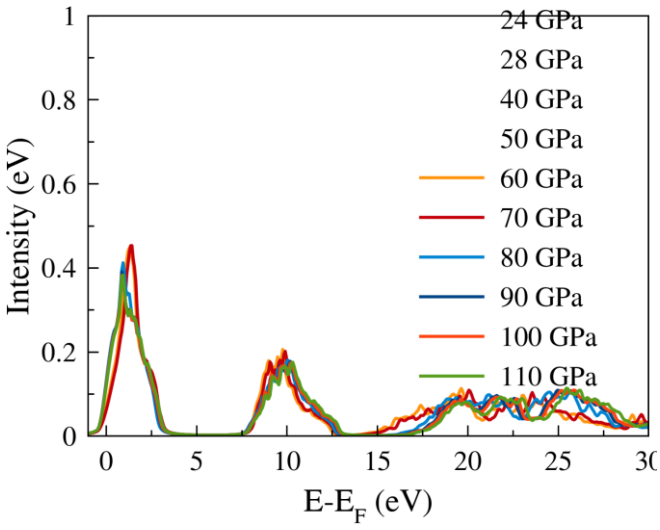

Figure 2. The XRS at pressure from 60 GPa to 110 GPa.

Figure 2 show the dependence of XRS in compression. The spectra change at 70-80 GPa indicating the phase transition from epsilon to zeta.

4. Conclusion

The calculated XRS are qualitatively comparable with room temperature XRS measurement at high pressure (>60 GPa). In the future we would like to use this method to calculate Silicate melts. We want to continue to use Hokusai system next year.

References:

[1] L. F. Lundegaard, G. Weck et al.: Nature, 443, 7108 (201-204) (2006).

[2] H. Peng, Z. H. Yang, J. P. Perdew, and J. Sun: Phys. Rev. X. 6, 041005 (2016).

[3] Y. Meng et al.: PNAS, 105(33) 11640-11644 (2008).

5. Schedule and prospect for the future

The XRS was considered as a promising feature to investigate the evolution of structures of materials in compression. The XRS together with first-principles molecular dynamics will be used in the future for crystals and melts. We want to continue to use Hokusai system next year.