EPSC Abstracts
Vol. 13, EPSC-DPS2019-556-1, 2019
EPSC-DPS Joint Meeting 2019

EPSC
EPSC-DPS Joint Meeting 2019
15–20 September 2019 | Geneva, Switzerland

B1-B2 Phase Transition in MgO from anharmonic *ab-initio* lattice dynamics at conditions of super-Earth interiors

Florian Trybel (1), Ion Errea (2,3), Donat Adams (4) , Michelle D. Wenz (5), Lorenzo Monacelli (6), Sergey Churakov (4), Matteo Calandra (7), Francesco Mauri (6,8), Raffaello Bianco (6,8,9), Daniele Passerone (10) and Gerd Steinle-Neumann (1)

(1) Bayerisches Geoinsitut, Universität Bayreuth, Bayreuth, Germany
(2) Donostia International Physics Center (DIPC), Donostia, Spain
(3) Fisika Aplikatua 1 Saila, University of the Basque Country (UPV/EHU), Donostia, Spain
(4) Institut für Geologie, Universität Bern, Bern, Switzerland
(5) Department of Earth and Planetary Sciences, Northwestern University, Evanston, IL, USA
(6) Dipartimento di Fisica, Università di Roma La Sapienza, Rome, Italy
(7) Sorbonne Universités, CNRS, Institut des Nanosciences de Paris, Paris, France
(8) Graphene Labs, Fondazione Istituto Italiano di Tecnologia, Genova, Italy
(9) Department of Applied Physics and Material Science, California Institute of Technology, Pasadena, CA, USA
(10) Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

Abstract

The B1-B2 phase transition in MgO near 500 GPa has been investigated in numerous experiments and numerical studies over the last decade. Nevertheless no consensus on the transition pressure and Clapeyron slope has emerged, and various model predictions spread over a wide pressure range. Here we present a numerical study of the transition using two lattice dynamics based approaches that include anharmonic and thermal effects.

1. Summary

The explosive growth in astronomical observations has revealed an unexpected variety of planetary bodies in the universe in terms of radius (R), mass (M) and orbital parameters. In order to characterize these exosolar planets, especially regarding the M-R relations, it is necessary to investigate phase stability fields of material candidates under conditions exceeding the temperature (T) and pressure (P) range of Earth's interior significantly. Especially the non-unique M-R ratios in the overlapping regimes of massive rocky planets (super-Earths) and small ice-giants (mini-Neptuns) complicate the classification in terms of interior structure and composition. The available high-T, high-P data and respective predictions of phase stability fields remain limited, as required P, T conditions are challenging not only in experiments, but also in simulations. In particular, the transition P and Clapeyron slopes of the $MgSiO_3$-ppv breakdown sequence in the MgO-SiO_2 system – proposed to dominate super-Earth mantles [1, 2] – are still not available to the precision necessary for the modelling of planetary interiors. Over the last decade numerous experimental [3, 4] and numerical [5, 6, 7] studies have investigated the B1-B2 transition in MgO as a prototype within the sequence, but the predictions for transition P and especially the Clapeyron slope still differ widely; in particular, a gap between experimental data and predictions from simulations exist.

In order to obtain temperature dependent transition pressures from density functional theory (DFT) based simulations, a thermal - or vibrational - contribution to energy (F_{vib}) must be added to the electronic ground-state energy. There it is possible to differentiate between two types of approaches: molecular dynamics (MD) and lattice dynamics (LD). In MD simulations the dynamics of the system is directly simulated by applying Newton's equation of motion using forces calculated from the electronic energies via application of the Hellmann-Feynman theorem. The vibrational contribution to energy can be calculated via thermodynamic integration. In this approach the T-dependence of F_{vib} is naturally incorporated, but thermodynamic integration requires a reference system, determining if anharmonic contributions are included. Furthermore the application of Newtonian dynamics is strictly valid

above the Debye temperature only, where all phonon modes are occupied. Therefore MD-based approaches suffer from limited applicability at low T.

In the framework of LD, on the other hand, phonon frequencies are calculated via linear response theory (e.g. ph.x of QUANTUM ESPRESSO [8, 9]) or the small displacement method (e.g. [10]) and F_{vib} from these phonon modes via occupation statistics. To date, the standard approach of including vibrational contributions to energy in LD simulations is to make use of the (quasi-) harmonic approximation, where a T-dependent F_{vib} is calculated through occupation of T-independent phonon modes calculated from harmonic force constants. Consequently, phonon-phonon interactions are not taken into account and thermal conductivity and expansion are not sufficiently described within the approximation. Using the harmonic approximation leads to a limited reliability at extreme conditions, as required for the simulation of the $MgSiO_3$-ppv breakdown sequence.

To overcome their respective problems, MD (e.g. [11]) as well as LD (e.g. [12, 13, 14]) based approaches have been under development that incorporate anharmonic effects, providing access to the invesitgation of phase stability fields and thermodynamic properties under extreme P and T conditions. We use the LD-based approaches SSCHA (stochastic self-consistent harmonic approximation) [13, 14] and DAMA (decoupled anharmonic mode approximation) [12] with QUANTUM ESPRESSO [8, 9] as the DFT-engine to include this type of corrections in our simulations regarding the B1-B2 phase-transition in MgO. Preliminary results show that the anharmonic contribution to F_{vib} leads to a shallower Clapeyron slope than previously predicted [3, 5], but in general agreement with recent predictions [15] using the MD-based approach [11].

Acknowledgements

This work is supported by DFG within the Research Unit FOR 2440 "Matter Under Planetary Interior Conditions". FT and GSN gratefully acknowledge computational and data resources provided by the Leibniz Supercomputing Centre (www.lrz.de) and sponsoring by NVIDIA through the "GPU Grant Program".

References

[1] D. Valencia, Physics and Chemistry of the Deep Earth, 271-294, 2013

[2] K. Umemoto, R. M. Wentzcovitch, S. Wu, M. Ji, C.-Z. Wang and K.-M. Ho EPSL 478, 40-45, 2017

[3] S. Root, L. Shulenburger, R. W. Lemke, D. H. Dolan, T. R. Mattsson, and M. P. Desjarlais, Phys. Rev. Lett. 115, 198501, 2015

[4] R. S. McWilliams, D. K. Spaulding, J. H. Eggert, P. M. Celliers, D. G. Hicks, R. F. Smith, G. W. Collins, and R. Jeanloz, Science 338, 1330, 2012.

[5] D. Cebulla and R. Redmer, Phys. Rev. B 89, 134107, 2014.

[6] S. A. Boates, B.and Bonev, Phys. Rev. Lett. 110, 135504, 2013.

[7] A. B. Belonoshko, S. Arapan, R. Martonak, and A. Rosengren, Phys. Rev. B 81, 054110, 2010.

[8] P. Giannozzi, et al., Journal of Physics: Condensed Matter 21, 395502, 2009

[9] P. Giannozzi, et al., Journal of Physics: Condensed Matter 29, 465901, 2017

[10] D. Alfè, Computer Physics Communications 180, 2622–2633, 2009

[11] O. Hellman, I. A. and Abrikosov and S. I. Simak, Phys. Rev. B 84, 180301, 2011

[12] D. Adams and D. Passerone, Journal of Physics: Condensed Matter 28, 305401, 2016

[13] I. Errea, M. Calandra, and F. Mauri, Phys. Rev. B 89,064302, 2014.

[14] R. Bianco, I. Errea, L. Paulatto, M. Calandra, and F. Mauri, Phys. Rev. B 96, 014111, 2017

[15] J. Bouchet, F. Bottin, V. Recoule, F. Remus, G. Morard, R. M. Bolis, and A. Benuzzi-Mounaix, Phys. Rev. B 99, 094113, 2019