Accepted Manuscript

Structural stability of FeO_2 in the pressure range of lower mantle

Mei Tang, Zhen-Wei Niu, Xiu-Lu Zhang, Ling-Cang Cai

PII: S0925-8388(18)32358-2

DOI: 10.1016/j.jallcom.2018.06.237

Reference: JALCOM 46573

To appear in: *Journal of Alloys and Compounds*

Received Date: 20 March 2018

Revised Date: 18 June 2018

Accepted Date: 19 June 2018

Please cite this article as: M. Tang, Z.-W. Niu, X.-L. Zhang, L.-C. Cai, Structural stability of FeO_2 in the pressure range of lower mantle, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.06.237.

Structural stability of FeO_2 in the pressure range of lower mantle

Mei Tang[2], Zhen-Wei Niu[1,*], Xiu-Lu Zhang[1], and Ling-Cang Cai[3]

[1]Laboratory for Extreme Conditions Matter Properties, Southwest University of Science and Technology, 621010 Mianyang, Sichuan, China

[2]Institute of Atomic and Molecular Physics, College of Physical Science and Technology, Sichuan University, Chengdu 610065, China;

[3] National Key Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang 621900, China

Abstract: Recently the finding of a new iron oxide pyrite-type FeO_2 is reported to involve in the oxygen cycles occurred in Earth's mantle. Understanding of the stability of FeO_2 at high pressures will be critical to model the cyclical process of oxygen in the lower mantle. Here we report the possible pressure-driven phase transition of FeO_2 in the pressure range of lower mantle by combining particle swarm optimization method and different density functional theory (DFT) techniques. We find a possible pressure-driven phase transition from PNNM symmetry phase to PA-3 symmetry (Pyrite-type) phase in the pressure range of lower mantle. Nevertheless, the stability of the PNNM symmetry phase is highly affected by temperature change. The possible pressure-driven phase transition is disappeared when the temperature exceeded 800 K. It is also found that the PNNM symmetry phase is mechanically unstable when temperature is beyond 800 K. Finally, the reactions Gibbs free energies of two possible decomposition reactions of FeO_2 are calculated from different DFT techniques. It is found that the pyrite-type FeO_2 decomposes to Fe_2O_3 and O_2 is the more likely scenario in the relative low-pressure and high-temperature region. However, more detailed calculations, where the phase transitions and the different spin state of iron oxides are also taken into account, are needed to clarify this decomposition reaction.

Keywords: pyrite-type FeO_2, elastic constants, structural stability, high pressure

PACS numbers: 62.20.Dc; 71.15.Mb; 91.35.-x

* Corresponding author. E-mail: z.w.niu@foxmail.com