

Poster Presentations

[MS20-P14] Experimental and theoretical equation of state of DyVO₄ polymorphs.

Wojciech. Paszkowicz^{a*}, Olga Ermakova^{ab}, Javier López-Solano^{c†}, Andrés. Mujica^c, Alfonso Muñoz^c, Romman Minikayev^a, Christian Lathe^{de}, Stanisław Gierlotka^f, Irina Nikolaenko^b, and Hanna Dabkowska^g

^aPolish Academy of Sciences, Institute of Physics, Warszawa 02-668, Poland.

^bRussian Academy of Sciences, Ural Branch, Institute of Solid State Chemistry (ISSC), Ekaterinburg 620219, Russian Federation.

^cDepartamento de Física Fundamental II, MALTA Consolider Team and Instituto de Materiales y Nanotecnología, Universidad de La Laguna 38205, Tenerife, Spain.

^dGeoForschungsZentrum Potsdam in der Helmholtz-Gemeinschaft, Department 5, D-14473 Potsdam, Germany.

^eHASYLAB at DESY, Notkestr., Hamburg 22607, Germany. ^fInstitute for High Pressure Physics, 01-142. Warsaw.

^gDepartment of Physics, McMaster University, Hamilton L8S 4M1, Canada. (†) current address, Izaña Atmospheric Research Center, Agencia Estatal de Meteorología (AEMET), 38071 Tenerife, Spain.

E-mail: paszk@ifpan.edu.pl

DyVO₄ is known for its Jahn-Teller type transition [1] and interesting magnetic properties [2]. A promising application for DyVO₄ is the catalysis in oxidative dehydrogenation of propane [3]. The DyVO₄/V₂O₅ mixture exhibits catalytic ability for decomposition of cyclohexanol [4] and strong photocatalytic activity in the decomposition of organics. A bismuth-containing solid solution, Bi_{0.5}Dy_{0.5}VO₄, has been found to be useful in photoinduced water splitting [5]. DyVO₄, like most of the RVO₄ family members, crystallizes in the zircon-type structure (I41/amd). At pressures in the range from 5 to 10 GPa, these compounds are known to undergo a phase transition into a scheelite-type polymorph (I41/a). The equation of state of a number of RVO₄ compounds has

been already determined, but not for DyVO₄. Regarding the phase transitions in DyVO₄, in [6] the scheelite-type phase was observed at pressures above 6.5 GPa. In a recent Raman spectroscopy study [7], the zircon phase was observed up to 8 GPa, followed by a zircon-scheelite phase mixture at 8.8 and 9.2 GPa, and single-phase scheelite at 10.7 GPa and above. The aim of the present investigation is to determine the yet unknown complete set of equation-of-state parameters for both dysprosium orthovanadate polymorphs, to experimentally check, whether the transition from the zircon phase to the scheelite phase occurs in the available pressure range and to provide the theoretical coexistence pressure. To achieve this goal, X-ray diffraction experiments and density-functional-theory (DFT) calculations are applied for the first time to the study of this material at high pressures. Furthermore, the DFT calculations allowed for the determination of the variation with pressure of the internal structural parameters of the unit cells and interatomic distances. To our knowledge this information was not previously available for DyVO₄ polymorphs. The present work provides the first diffraction based experimental information on elastic properties of zircon-type and scheelite type dysprosium orthovanadates. The obtained experimental data compare well with the (first) theoretical DFT-based results. Namely, the bulk modulus equals 118 GPa (experimental) or 126 (theoretical) for the zircon phase, and equals 153 (experimental) and 142.9 (theoretical) for the scheelite phase. The good agreement supports the reliability of both, experimental and theoretical data obtained. Moreover, the quoted values are close to one of early evaluations for DyVO₄, 126 GPa, and to those experimentally determined for some other RVO₄ compounds.

Acknowledgements: Partial support of the European Community in the frame of European Action towards Leading Centre for Innovative Materials (Eagle) REGPOT-2012-2013-1, EU FP7 is gratefully acknowledged.

- [1] Vekhter, B.G., Kaplan M.D. (1979) *JETP Lett.* **29**, 155-157.
- [2] Sieger, M., Kasten, A. & Paul, W. (1985). *Solid State Commun.* **53**, 909-913.
- [3] Au, C.-T. & W.-D. Zhang (1997) *J. Chem. Soc., Faraday Trans.* **93**, 1195-1204.
- [4] Sugunan, S. & Renuka, N.K. (2002) *Indian J. Chem.* **41A**, 692-700.
- [5] Wang, Q., Liu, H., Jiang, L., Yuan, J. & Shangguan, W. (2009) *Catal. Lett.* **131**, 160-163.
- [6] Duclos, S.J., Jayaraman, A., Espinosa, G.P., Cooper, A.S., & Maines Sr., R.G. (1989) *J. Phys. Chem. Solids* **50**, 769-775.
- [7] Patel, N.N., Garg, A.B. Meenakshi, S., Wani, B.N. & Sharma, S.M. (2010) *AIP Conf. Proc.* **1349**, 99-100.

Keywords: pressure, structure refinement, ab initio calculations.