

**MULTIPHASE EQUATIONS OF STATE FOR PLANETARY IMPACT STUDY -II.** B.A Ivanov, Institute for Dynamics of Geospheres, RAS (Lenynsky Prospect 38-1, 119334 Moscow, Russia, baivanov@idg.chph.ras.ru).

**Introduction:** Impacts of comets and asteroids play an important role in geologic evolution of terrestrial planets (e.g. [1]). Impact related processes operate in a wide range of pressures and temperatures. Impact modeling inherently needs equation of state (EOS) for rock forming minerals and various rocks.

One of approaches to improve EOS for rock-forming materials is to apply computer-supported EOS'es (like ANEOS [2]) to describe restricted phase space areas as an independent material with following determination of phase boundaries (like in PANDA [3, 4]). Previously we have made some preliminary tests of this approach in application to a few geomaterials and H<sub>2</sub>O [5-7]. In the previous conference we presented first data for fayalite Fe<sub>2</sub>SiO<sub>4</sub> [8]. Here we present the first results for forsterite Mg<sub>2</sub>SiO<sub>4</sub>.

**EOS construction:** The EOS construction is started with fitting parameters for 4 materials modeling forsterite melt, low pressure phase and 2 high pressure phases. As the closest goal of the project is to improve rock melting description in high-velocity impact modeling we simplify the intermediate zone of high pressure phases coexisted near 20 GPa assuming the assemblage as one material. ANEOS code is used to compute equations of state of each material in the current 4-material model. ANEOS options of melting and solid-solid phase transitions are switched off. Phase boundaries are searched from thermodynamic equilibrium conditions.

The simplest way to fit experimental data is used: the equilibrium at the normal pressure at the melting temperature and in the first triple point allows us to find values of energy and entropy shift between lpp and melt. Equilibrium in the first triple point between melt, lpp, and hpp-1 defines the energy and entropy shift for hpp-1. The same procedure is repeating for the second triple point. The quality of the constriction is immediately checked with calculation of lpp/hpp-1 and hpp-1/hpp2 phase boundaries construction.

Fig. 1 shows model phase boundaries in comparison with experimental data below ~20 GPa the phase space geometry is well reproduced. However, the hpp-1/hpp-2 phase boundary has less steep inclination than the experimental boundary. Partially the deviation may result from omitting of intermediate phases in the model hpp-1 area.

Another way to verify the model is to compare individual properties of phases with experimental data. For melts wide range data are rare, and we use also results of molecular dynamic models. Fig.2 illustrate

the compressibility of model melt along isotherm T=3000K with MD forsterite model [11]. Above ~20 GPa the simple ANEOS model reasonably well repeat the MD results.

**Discussion:** The constricted EOS is easy to use for compilation of standard tables readable in a hydro-code. Some changes are needed to describe fraction of complete melt along the melt temperature. The presented approach promises more robust description of melt production what is important for models of giant impacts on early (hot) terrestrial planets. However monomineral models for fayalite [8] and forsterite (this work) separately do not reproduce liquids/solidus behavior typical for real mantle dunites. Hence the next step of the project should include the description of solid solutions to produce a workable mantle model.

Another model extension we plan to test is the presentation of melt as a mixture of melts with low and high coordination number (presented in ANEOS-like models with different density and compressibility). For example, Ghiorso [12] uses the mixture of 5 to 6 silicate liquids with consequently increasing coordination number and make a smooth transition in liquid properties from low to high pressures. This approach potentially may improve the melt curve for high pressure looking too steep in the presented model (Fig. 1).

**References:** [1] Melosh H. J. (1989) *Impact Cratering*. Oxford, 245 pp. [2] Thompson, S. L., Lauson, H. S. (1972) *Sandia National Laboratory Report SC-RR-71 0714*. [3] Kerley, G. I. (1991) *Sandia Report SAND88-2291*, Albuquerque, NM., 176 pp.. [4] Kerley G. I. (1989.) *High Pressure Res.* 2, 29-47. [5] Ivanov B. (2003) in *Impact Cratering: Bridging the Gap Between Modeling and Observations*, abstr. #. 40. [6] Ivanov B. et. al. (2004) *LPSC35th*, abs. #1489. [7] Ivanov B. (2005) *LPSC36th*, abs. #1232. [8] Ivanov B. (2008) *LPSC39th*, abs #1490. [9] Navrotsky A. (1995) In: *Handbook of Physical Constants, AGU Reference Shelf 2*, p. 17-28. [10] Davis B.T.C. and J.L. England (1964) *JGR* **69**, 1113-1116. [11] de Koker N.P et al. (2008) *GeoCosmoActa* **72** (5), 1427-1441. [12] Ghiorso, M. S. (2004) *Am. J. Sci.*, 304, 752-810.

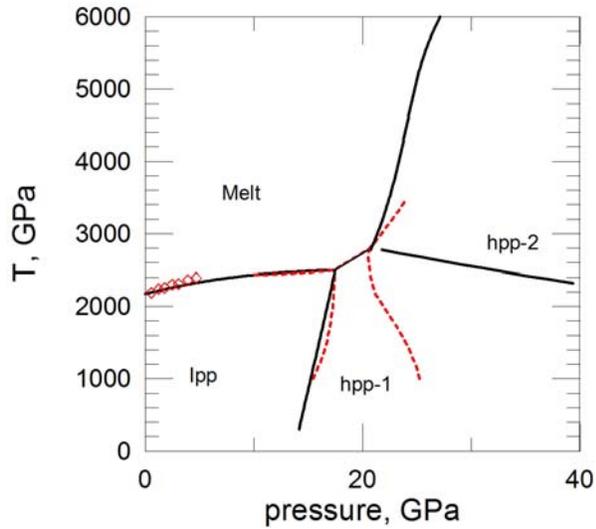


Fig. 1. Phase boundaries for the simplified forsterite model (black curves) computed for 4 ANEOS-based materials (low pressure phase, lpp, intermediate high pressure phase, hpp-1, perovskite high pressure phase, hpp-2, and melt). Boundaries are constructed for the thermodynamic equilibrium. The main experimental phase boundaries (dashed red lines) are plotted after [9]. Experimental data for low pressure [10] are presented with red open diamonds.

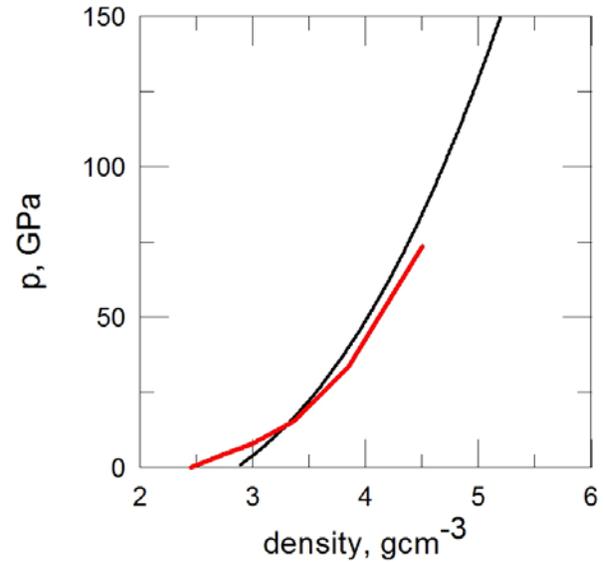


Fig. 2. Pressure vs. density for the model liquid phase (black curve) at  $T=3000\text{K}$  in comparison with results of molecular dynamic modeling (red curve) after [11].