MULTIPHASE EQUATIONS OF STATE FOR PLANETARY IMPACT STUDY. B.A Ivanov, Institute for Dynamics of Geospheres, RAS (Leninsky 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]). In addition to primary space mission data (imagery, radar reflection and gravity anomaly measurements, returned samples, Martian meteorites), modeling of natural processes is now a powerful technique of data analysis. 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. Many very useful EOS'es have been constructed in last decades for specific phase space zones (e.g. – along experimentally derived Hugoniot curves). However the numerical modeling of high velocity demands to have smooth description of various states of material (from super-compressed solids to rarefied impact vapors). In addition, numerous important solid-solid phase transitions in rocks often complicate accurate description of important parameters such as post-shock temperatures and partial and complete melting).

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_20 [5, 6]. Here we present preliminary data for one more rock-forming mineral – fayalite Fe_2SiO_4.

Rock EOS'es: The last decades ANEOS (computer-supported analytical equation of state) is widely used to simulate typical geomaterials such as granite dunite, and basalt. In many computer models these materials are in use as the best available proxies for crustal and mantle materials on different planetary bodies. However in the current state ANSOS is unable to treat simultaneously solid-solid phase transition (only one transition is affordable) and melting. Constructing H_20 ANEOS-based EOS [7] the liquid phase (water) is described as a separate material. This approach allows us to reproduce negative slope of $T_{melt}(p)$ for water/iceIh phase boundary.

Similar presentation of quartz main phases (quartz, coesite, stishovite) is used to reproduce static phase diagram for $Si0_2$ [6]. However in [6] melting of each phase is described with the standard ANEOS melting routine. While phase boundaries in solid state and melting curves are well reproduced, phase boundaries are continued into liquid state creating unnatural sharp phase boundaries between melts of different states. It is known that the good representation of experimental and molecular dynamics modeling data is achieved providing the gradual change in the coordination number of molecules in liquids. Hence we need to add a similar approximate description to the ANEOS-based equation of state for liquids. Here we investigate the possibility to use one model liquid to present EOS for fayalite up to 15 GPa.

Fayalite – First Step: Recently published analytical equations of state for fayalite [13, 14] considerably facilitate collection and comparison of available experimental data. Following [13, 14] we have fitted ANEOS for 5 materials presenting individual phases: liquid, low pressure α-phase, high pressure γ-phase (spinel), and post-spinel phases (assumed, after [10, 13, 14], to be a mixture of FeO and SiO_2.

We meet considerable problems to merge a mixture EOS for FeO and SiO_2 together with first 3 phases due to problems in the field of coexistence of the liquid FeO and solid stishovite. The coexistence of molten FeO below the liquidus and the model total melt above the liquidus addresses us to the question how to present EOS for molten silicates. For example, Ghiorso [15] 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. In contrast, Mosenfelder, Asimow, and Ahrens [16] discuss the possibility of phase transition boundaries in the molten forsterite. The probem is under investigation.

First results of the ANEOS-based description of fayalite are presented below. Fig. 1 illustrates the first triple point between melt and α and γ solid phases. Despite the simplicity of principles used in ANEOS, the melting curve behavior to ~20 GPa is similar to experimental data and published analytical EOS'es for fayalite [13, 14].

The liquid phase of the model fayalite without phase transitions gives the Hugoniot curve close to experimental data [10] covering the pressure range to ~50 GPa.

The price of the ANEOS usage is the very approximate reproduction of melt density and compressibility at normal pressure (Fig. 3). The model curve is going below published experimental data and gives too steep decrease of the bulk compression modulus in a hot liquid. In addition, the melt density at the boiling point (calculated as ~2830 K at 1 bar) decreased below

2 g cm^{-1}. However, the general behavior of the liquid below 20 GPa looks reasonably enough.

Conclusions: The advantage of ANEOS like equations of state is the easiness of a smooth extrapolation to high pressure and temperature fields where no experimental data exists. To use this feature we need to take a lot of efforts to fit the model to the experimental data. The progress promises us more reliable results in the numerical modeling of large-scale planetary impacts.

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] Akimoto S. et al. (1967) *JGR, 68,* 679-686. [9] Ohtani E. (1979) J. Phys. Earth 27, 189-208. [10] Chen, G. Q. et al. (2002) *Phys. Earth Planet. Inter., 134*, 35-52. [11] Rivers and Carmichael (1987) *JGR, 92*, 9247-9270. [12] Lange and Carmichael (1987) *Geochim. Cosmochim. Acta, 51*, 2931-2946. [13] Fabrichnaya O. B. and B. Sundman (1997) *Geochim. Cosmochim. Acta, 61*, 4539-4555. [14] . Jacobs M. H. G. et al. (2001) *Geochim. Cosmochim. Acta, 65*, 4231-4242. [15] Ghiorso, M. S. (2004) Am. J. Sci., 304, 752-810. [16] Mosenfelder J. L. et al. (2007) *JGRB, 112*, doi:10.1029/2006JB004364.

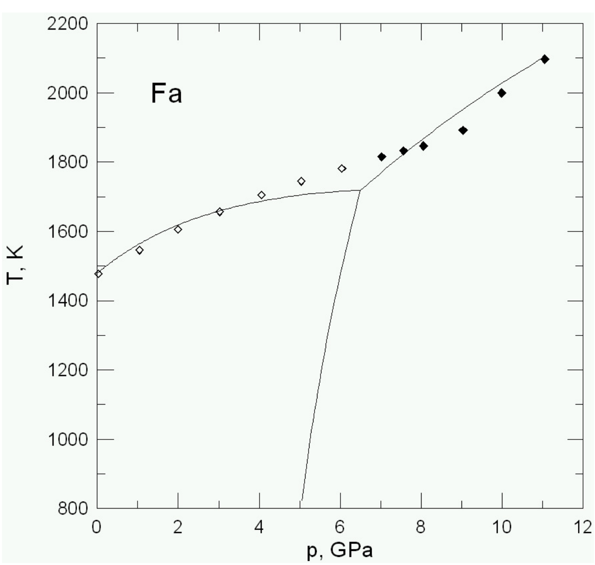

Fig. 1. Triple point of melted fayalite, low-pressure solid α-phase and the high-pressure solid γ-phase. Solid curves are equilibrium lines constructed with the ANEOS-based equation of state. Experimental data [8, 9] are shown as open diamonds for the α-phase melting and as filled diamonds for γ-phase melting.

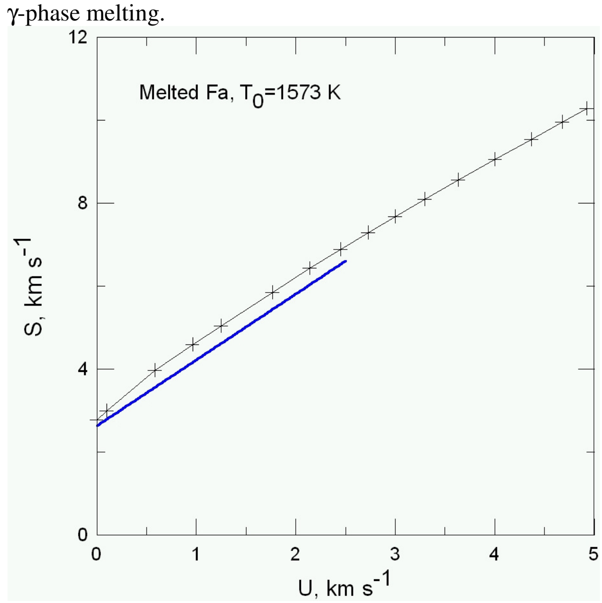

Fig. 2. Comparison of the model Hugoniot curve for the molten fayalite in S-U coordinates (shock velocity – particle velocity, shown as the curve with small crosses) with the linear approximation of experimental data [10]. Experimental data cover the pressure range up to ~50 GPa for the initial density shown in Fig. 3.

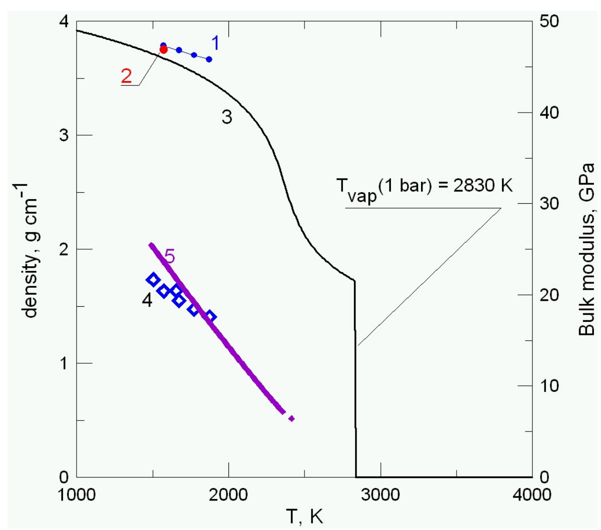

Fig. 3. Some details of the quality of the ANEOS-based equation of state for molten fayalite at normal pressure (1 bar). Experimental points for density vs. temperature: 1 - [12], 2 – [10], 3 – this work (left scale bar); Bulk modulus (right scale bar): 4 – [11, 12], 5 – this work. Model boiling temperature at 1 bar pressure is ~2830 K.