European Mineralogical Conference
Vol. 1, EMC2012-103, 2012
European Mineralogical Conference 2012


# Experiments vs. Databases - Phase Equilibria in the System Glc, Plg, Cpx, Qz and Tc.

M. Zaehle (1), E. Duesterhoeft (1), R. Bousquet (2), and R. Oberhänsli (1)

(1) Institute of Earth and Environmental Science, University of Potsdam, Potsdam, Germany (mzaehle@uni-potsdam.de), (2) Geosciences Rennes, Université Rennes 1, Rennes, France

In times of modelling geodynamic processes through thermodynamic equilibria, the system Glc, Plg, Cpx, Qz and Tc is the describing system for mafic blueshist-rocks. Here, glaucophane is the determining index mineral. Its maximum stability is of great diversity regarding well accepted literature. In 1983, Carman & Gilbert determined the highest stability to be at around 800°C and 36 kbar and the reaction of Glc = Jd + Tc to have a positive slope. In 1988, Holland & Powell determined the stability to be over 40 kbar at lower temperature and the reaction to have a negative slope, resulting in a field of uncertainty that is half the size of the biggest proposed stability-field itself. Additionally, the newest data of Jenkins & Corona point out that the upper stability of glaucophane is similar to that proposed by Carman & Gilbert. While amphiboles are probably the toughest minerals to be modeled because of their variety and complex solid solutions, it should be clear that glaucophane is the most important one in understanding the evolution of mafic blueshist-rocks whereas the correct calculation of its volume is of great significance when modelling subduction zones.
Mineral volumes are a complex matter in the field of thermodynamic modelling and an important physical property in geodynamic processes. As a major factor in the calculation of phase equilibria based on the Gibbs free energy minimization, mineral volumes can help to estimate the reliability of thermodynamic databases, especially in cases of great uncertainty. With the help of the newest version of Theriak/Domino, we investigate the calculated volumes of the involved minerals using the database of Berman (1988) with the addition of Evans (1990) and the database of Holland & Powell from 1998 (as we show, based on an incorrect Landau-transition term) and 2011 (now with the correct transition term) in comparison to available experimental data. Not only are there notable differences in the methodology used but also in the resulting places of mineral reactions, volumetric behaviour and therefore the geodynamic implications. By evaluating thermodynamic databases, pointing out discrepancies, we hope to create some awareness in the use of well established datasets. It is made obvious that newer datasets are not necessarily better than older ones, when it comes to the calculation of mineral volumes and phase equilibria.
Despite the fact that mineral volumes can be well determined by experiments, some methods fail to predict correct volumes under high pressure and temperature conditions. In a novel and relatively simple approach, the existing volumes of Berman's database from 1988 can be improved to provide higher correspondence to experiments under elevated conditions, ultimately making them equal or better than the ones of Holland & Powell's database in quite a few circumstances. As the volumetric behaviour of minerals as well as their stability plays a significant role as a driving force in subductional processes, it is our goal to improve the base of knowledge on these utterly important features based on existing data.

Further Reading:

[1] Carman & Gilbert (1983), Experimental studies on glaucophane stability, Journal of Science.

[2] Holland (1988), Preliminary phase relations involving glaucophane and applications to high pressure petrology: new heat capacity and thermodynamic data, Contributions to Mineralogy and Petrology.

[3] Berman (1988), Internally-Consistent Thermodynamic Data for Minerals in the System Na2O-K2O-CaO-MgO-FeO-Fe2$O_3$-Al2$O_3$-$SiO_2$-$TiO_2$-$H_2O$-$CO_2$, Journal of Petrology.

[4] Evans (1990), Phase relations of epidote-blueshists, Lithos.

[5] Holland & Powell (1998), An internally consistent thermodynamic data set for phases of petrological interest, Journal of metamorphic Geology.

[6] Jenkins & Corona (2006), Molar volume and thermal expansion of glaucophane, Physics and Chemistry of Minerals.

[7] Jenkins & Corona (2010), Compressibility of synthetic glaucophane, Physics and Chemistry of Minerals.

[8] Holland & Powell (2011), An improved and extended internally consistent thermodynamic dataset for phases of petrological interest, involving a new
equation of state for solids, Journal of metamorphic Geology.

[9] Duesterhoeft, Zaehle, De Capitani, Oberhänsli & Bousquet (2012) submitted to Contributions to Mineralogy and Petrology.