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The influence of thermodynamic databases on the lithospheric density

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Thermodynamic databases are an essential tool to predict complex equilibrium mineral assemblages and mineral properties like density. They consist of numerous thermodynamic data of various minerals, extracted from experiments. Each database follows its own methodology in calculating chemical and physical properties. Recently, many studies are focusing on modeling physical properties like density or seismic velocity using thermodynamic software packages like Perple_X, Theriak-Domino or Thermocalc. Therefore, it is more topic than ever to investigate the influence of thermodynamic databases on these parameters and the resulting geodynamic predictions.

Here, we focus on (here called) "metamorphic density" calculations of the crust and lithospheric mantle predicted by different thermodynamic databases. We developed a one-dimensional model, which calculates metamorphic density as a function of pressure, temperature, and chemical composition, based on the fact that the geothermal gradient in the lithosphere and crust influences the density distribution. This is a new petrologic aspect, because (here called) "physical density" models generally do not take into account the effects of metamorphic phase transitions and ignore the fact that chemical reactions influence both, the stability of mineral assemblages and rock density. We compare the metamorphic densities (predicted by different databases) with each other and with the physical density (taking no mineralogical changes into account). Our model underscores how metamorphic density of the lithosphere varies with depth and reveals how the combination of chemical composition of rocks, mineralogy, and geothermal gradient all have significant effects on the density distribution within the lithosphere. Thus, we show that metamorphic phase transitions in crust and lithospheric mantle have an influence on its density distribution and show that physical density models that ignore metamorphic processes and/or mineral reactions are no longer representative of the density distribution in the crust and lithosphere.

Our results are very instructive and suggest that the input three layer composition model, consisting of upper crust, lower crust and lithospheric mantle results in an up to 6 layer density model, due to significant mineralogical changes. Nevertheless, there are discrepancies between the metamorphic density predictions, in consequence of different database methodologies. We show that rock-density can vary significantly by changing the thermodynamic database. This density difference is dramatic and must be considered, keeping in mind that the database are both founded on experiments of well studied minerals (e.g. quartz or forsterite). These discrepancies between the databases impact geodynamic interpretations, due to the fact that the achievement of topography is first driven by density variations in the earth. Nevertheless, calculating the density considering mineralogical changes is a clear improvement compared to physical density models. Summarizing, reliable volumes are necessary to calculate volume dependent physical properties like density or seismic velocity. It is important to estimate the influence of the thermodynamic database on Gibbs free energy, volume and rock density. Therefore more experimental data will lead to a better comprehension of the discrepancies between thermodynamic databases.

Further Reading:

[1] Duesterhoeft, Bousquet, Wichura & Oberhänsli (2012), submitted to Journal of Geophysical Research

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