

Modeling phase equilibria in FMAS with regard to UHT-metamorphism

K. K. Podlesskii (1,2)

(1) Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry (IGEM), Russian Academy of Sciences, Staromonetny per. 35, 119017 Moscow, Russia (kkp@igem.ru), (2) Institute of Experimental Mineralogy, Russian Academy of Sciences, 142432 Chernogolovka, Moscow region, Russia (kkp@iem.ac.ru)

Phase equilibria in the system FeO-MgO-Al₂O₃-SiO₂ (FMAS) involving garnet, orthopyroxene, spinel, olivine, cordierite, sapphirine, alumina silicates, corundum and quartz have been calculated with different internally consistent thermodynamic datasets. The results show significant discrepancies between the stability fields of mineral assemblages indicative of UHT-metamorphism. Typology of the derived PT-grids and behavior of the solid solutions demonstrate severe dependence on the dataset used and allow too much freedom of interpretation. Being insufficiently constrained by measurements and experimental data, the standard thermodynamic properties of end-member minerals and mixing properties of solid solutions may give rise to estimates that cannot be considered confident. Even phase relations in the subsystems FAS and MAS cannot be described unambiguously in terms of both the grid typology and PT-values. Lack of reliable experimental data on changes in composition of sapphirine with temperature and pressure inevitably requires considerable ambiguity in modeling reactions involving this mineral. Experimental data also do not provide sufficient constraints for extrapolating properties of iron-bearing orthopyroxene into the range of composition with high alumina contents typical for UHT-granulites. The discrepancy between estimates of the aluminous orthopyroxene stability boundary in the system FAS calculated with different models may exceed 100°C. While employing modern software packages for interpreting natural processes, it is worth remembering that the thermodynamic data that form their basis are far from perfect and can hardly be improved without additional experimental work.

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