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Fast effective Bulk Composition-projected Phase Diagram Calculations

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Rare Moldanubian rocks associated with peridotites are characterized by garnet porphyroblasts (< 3 cm) within a texturally well-equilibrated, quartz-free matrix composed of plagioclase, hornblende, clinopyroxene of varying modal amounts. Bulk analyses of these rocks show unusual peraluminous mafic compositions characterized by normative corundum contents as high as 14%. The garnet (Grt) porphyroblasts enclose large kyanite (Ky) crystals and show a pronounced Mg and Ca rich composition (X_{Fe} = 0.24, X_{Mn} = 0.01, X_{Mg} = 050, X_{Ca} = 0.25) with flat element distributions. These distributions are disturbed within reactive garnet domains present at the garnet rim, along symplectite-filled cracks and around Ky inclusions.

Extensive analytical and textural analysis with the microprobe show that within reactive domains the garnet (a) partially brakes down to numerous types of symplectites and (b) adjusts locally its composition by diffusion. The symplectites may contain corundum (Crn), clinopyroxene (Cpx), orthopyroxene (Opx), hornblende (Hbl), plagioclase (Pl), sapphirine (Spr) and spinel (Spl). Tab. 1 shows the various symplectite types and reactive domains of Grt. The striking features of the minerals may be summarized as follows: (1) Irrespective of its occurrence, the Cpx has negligible jadeite, but occasionally high CaAl-pyroxene contents (<22 mol-%). (2) the Hbl is characterized by appreciable tschermakite contents (<17 mol-%). (3) the Pl may occasionally be close to pure anorthite. (4) Spr and Spl are Al and Mg rich. These features reflect the unusual Al, Mg and Ca rich composition of the rocks.

Table 1: Symplectite types and reactive domains of garnet.

Symplectite type	**Grt domain**
Spr+Pl+Opx+Spl	Rim
Opx+Spl+Pl+Hbl	Rim
Crn+Spl+Spr+Pl	Crack
Spl+Opx+Pl	Crack
Cpx+Opx+Spl enclosed by Hbl+Pl	Crack
Crn+Pl followed by Spr+Pl	Ky inclusions

Textural evidence suggests that Grt + Ky first broke-down to Crn + Pl $\pm$Spl and then to Spr $+$ Spl + Pl symplectite. Similarly, Cpx + Opx + Spl has been followed by symplectites of Hbl + Pl. The overall rock evolution is characterized by high-temperature decompression of the rocks.

Combined with the compositional readjustment of Grt observed within the reactive domains, the various symplectite types, as well as the chemical variability of the same mineral among the reactive Grt domains suggest that symplectite formation may have been controlled not only by pressure, temperature and time, but also locally by (effective) bulk composition. This further suggests that application of conventional thermobarometric methods will probably provide unreliable constraints for estimating the *PT* evolution of the rocks.

The alternative technique is to calculate (effective) bulk composition-projected *PT* phase diagrams (pseudosections) that may help estimate the *PT* trajectory of the rock by fulfilling the objectives of reproducibility (a) of the observed type and sequence of symplectites and (b) the observed mineral compositions. Generally, this approach involves some trial and error and can be extremely time-consuming without granting success. Straightforward application is granted by software that is based on fast-computing algorithms and has the ability to calculate and plot “ready to use” phase diagrams in reasonably short times without user intervention. These requirements are met optimally and elegantly by the Theriak/Domino software package, multi-platform (Unix and derivates, Mac, PC) version 301204 (de Capitani & Brown, 1987).

Nevertheless, even the best software cannot overcome problems arising from missing or unconfident thermodynamic data. In case of the rocks discussed here, this problem is related to mixing models appropriate for the observed Ca-Al rich pyroxenes as well as confident standard data for sapphirine. The Theriak/Domino software is capable of computing with the thermodynamic databases (standard data and mixing models) of Berman (1988), Berman & Aranovich (1996) (dataset 1) as well as Holland & Powel (1998) (dataset 2).

Using the Theriak/Domino software, “compromised” standard data for Spr available in the literature and ideal site mixing for Spr and Cpx, bulk composition-projected phase diagrams as well as isopleths of mineral compositions were calculated and plotted using both datasets for comparison. For the latter tasks, less than 14 minutes per “ready to use” diagram are needed with a modern PC. The results are strikingly similar and fulfill the objectives mentioned earlier. They can be summarized as follows.

1. The observed relations are the result of overall rock decompression in the range 15 to 8 kbar at temperatures around 750˚C. Earlier stages that might have been characterized by jadeite richer Cpx are not documented by the data, but are not excluded.

2. The calculated initial assemblage is Grt+Cpx+Ky. This is consistent with the observed Ky and Cpx inclusions in Grt, however, the calculated Cpx composition has higher jadeite contents (ca. 15%). Such Cpx compositions have not been observed because, obviously, have not survived the decompression.

3. The instability of Grt+Ky during decompression controls the formation of the earliest symplectites in most reactive domains.

4. Fe, Mg and Ca isopleths corresponding to the homogenized composition of the Grt porphyroblasts cross each other surprizingly at a point suggesting homogenization/ equilibration conditions at ca. 12 kbar and 750˚C.

5. The trajectory reproduces the observed sequence in the development of the symplectite types.

6. The results are consistent with earlier independent thermobarometric results from simpler Moldanubian rocks (Petrakakis, 1997).

The Theriak/Dominos software is an easy to use, fast-calculation and plotting tool that helps analyze complex paragenetic relations in rocks, and assists checking and adjusting the available thermodynamic data towards their consistency with nature.

References

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