**Supplementary material (B31040 - Álvarez-Valero et al.)**


**Determining bulk compositions**

Whole rock bulk analyses for anatectic rocks have limited use for phase diagram modeling because each microdomain may represent a different melting **"equilibrium"** stage (different equilibrium volumes sensu stricto Stu we, 1997) within the same rock (or thin section). Therefore, the melting evolution is investigated using discrete modal bulk compositions, calculated from local mineral modes and composition, instead of bulk rock XRF analysis, to avoid the construction of unreliable pseudosections. In most cases a pre-existing porphyroblast is inferred to be in reaction relationship with its surrounding matrix, and exchanging material with it. A local bulk composition can be determined by estimating the volume proportions of phases in a domain centred on the porphyroblast and extending out into the host matrix to define a volume (ideally the smallest such volume) that could be considered closed to non-volatile components. The modal proportions were determined mainly by image analysis of microphotographs or backscattered electron images, supported by visual estimation. The mean compositions for all phases are determined, summed according to their volume proportions, and finally expressed as molar percentages of oxide components in the system NCKFMASHT.

This is a moderately objective approach that does not presume a prior knowledge of the reaction process beyond what can be established by petrographic observation. However, it is subject to certain qualifications and uncertainties. The most important of these relates to divergence between the total bulk composition and the effective bulk composition (cf. Stüwe, 1997), i.e. the part of the system that was in full chemical communication and approached a state of equilibrium at the P and T of interest. This divergence may arise from disequilibrium, for example a resorbing porphyroblast whose interior is out of equilibrium with surrounding phases, or from growth zoning of new phases leading to fractionation of the effective bulk composition. The discrepancies are minimised if compositional zoning is minor and if relict cores (of garnet, for example) are of small volume and similar in composition to equilibrated rims. In practice, the principal zoning in garnet is in the MnO content, varying over about 2

wt%, largely compensated by FeO. A mean composition, weighted towards that of the rims, was used for the bulk composition calculation. In view of the minor compositional zoning and the small volume contribution from fractionated grain cores, we did not adjust the estimated bulk compositions for this effect.

A second factor is that the estimated bulk composition depends on a somewhat arbitrary choice of outer boundary for the system. This choice does not significantly affect the P–T determination, which relies on matching the observed and calculated phase compositions and modes in whatever system has been defined. However, since it does affect the size of the matrix reservoir, it may have a second-order effect on the predicted changes in mineral proportions and compositions across assemblage fields towards the final P–T condition, and on the position of high-variance field boundaries.

A third effect is related to the geometry of the local domains. The true equilibration volume about a reacting or growing porphyroblast may be roughly spherical, whereas mode estimates are based on area measurement in thin section. An area estimate over-weights the contribution from a porphyroblast core, and under-weights the matrix envelope, relative to the likely volume contributions.

The sensitivity of field boundaries on the calculated diagram to uncertainty in the bulk composition depends on the variance of the assemblage: low-variance assemblages are insensitive; high-variance assemblage boundaries more uncertain.

The involved phases in the model: Grt, Crd, Spl, Bt, Sil, Ky, Pl, Kfs, Ilm, Ru, Qtz and silicate liquid (M). Inclusions of rhyolitic composition are found in both the higher and lower P assemblages in Grt, Ky, Pl, Zr, and Crd crystals, and hence are interpreted as fresh glass. The model for silicate melt, as well as activity–composition models or Grt and Bt, is taken from White et al. (2007); for Spl and hydrous Crd from Holland and Powell (1998); and for feldspars from Fuhrman and Lindsley (1988). The activity–composition model for Bt is from Tajcmanová et al. (2009). The model biotite is saturated in Ti by incorporating enough $TiO_2$ to allow excess ilmenite.

The following series of tables lists, for each modeled material, the input compositional data and the results of the model calculations. Input data consist of the simplified phase compositions in NCKFMASHT and their estimated volume proportions. The listing of results consists of calculated phase compositions and volume proportions at the conditions chosen as the best match with the observed assemblage or reaction process.

**Modeled material: Grt growth from Bt incongruent melting (Fig.3A)**

observed phase compositions and volume proportions, based on specimen BB-11-56

|          | Garnet | Biotite | Plagioclase | K-feldspar | Melt |
|----------|--------|---------|-------------|------------|------|
| Si       | 2,99   | 2,72    | 2,56        | 2,98       | 3,69 |
| Ti       | 0,00   | 0,28    | 0,00        | 0,00       | 0,00 |
| Al       | 2,08   | 1,44    | 1,43        | 1,02       | 0,23 |
| Fe       | 1,78   | 0,66    | 0,00        | 0,00       | 0,08 |
| Mg       | 0,82   | 1,71    | 0,00        | 0,00       | 0,08 |
| Ca       | 0,26   | 0,00    | 0,37        | 0,01       | 0,00 |
| Na       | 0,00   | 0,03    | 0,57        | 0,16       | 0,00 |
| K        | 0,00   | 0,90    | 0,01        | 0,82       | 0,10 |
| H        | 0,00   | 2,00    | 0,00        | 0,00       | 0,64 |
| $X_{Fe}$ | 0,68   | 0,28    |             |            |      |
| Vol %    | 20,0   | 12,0    | 17,0        | 20,0       | 7,0  |
| (includes 12% kyanite, 12% quartz) | | | | | |

calculated phase compositions and volume proportions at 750 ±50°C, 11 ± 1 kbar

|          | Garnet | Biotite | Plagioclase | K-feldspar | Melt |
|----------|--------|---------|-------------|------------|------|
| Si       | 3,00   | 3,00    | 3,00        | 3,00       | 3,40 |
| Ti       | 0,00   | 0,00    | 0,00        | 0,00       | 0,00 |
| Al       | 1,00   | 0,50    | 0,50        | 0,50       | 0,42 |
| Fe       | 1,44   | 0,79    | 0,00        | 0,00       | 0,00 |
| Mg       | 0,69   | 2,21    | 0,00        | 0,00       | 0,00 |
| Ca       | 0,77   | 0,00    | 0,50        | 0,00       | 0,03 |
| Na       | 0,00   | 0,00    | 0,50        | 0,20       | 0,24 |
| K        | 0,00   | 0,50    | 0,00        | 0,80       | 0,13 |
| H        | 0,00   | 1,00    | 0,00        | 0,00       | 0,70 |
| $X_{Fe}$ | 0,68   | 0,26    |             |            |      |
| Vol %    | 17,7   | 16,1    | 12,0        | 7,7        | 12,2 |
| (includes 8.3 % kyanite, 25 % quartz, 1 % rutile) | | | | | |

Note: Best match as determined by $X_{Fe}$ nearness of Grt and Bt and isomodes intersection.

**Modeled material: Spl+Crd+M+Pl coronas on both alumino-silicate and Grt (Fig.3B)**

observed phase compositions and volume proportions, based on specimen BB-11-56

| | Garnet | Spinel | Cordierite | Biotite | Plagioclase | K-feldspar | Melt |
|---|---|---|---|---|---|---|---|
| Si | 2,98 | 0,00 | 5,00 | 2,76 | 2,61 | 3,00 | 3,18 |
| Ti | 0,00 | 0,00 | 0,00 | 0,16 | 0,00 | 0,00 | 0,00 |
| Al | 2,08 | 1,99 | 4,02 | 1,48 | 1,41 | 1,00 | 0,86 |
| Fe | 1,96 | 0,80 | 0,78 | 1,05 | 0,00 | 0,00 | 0,02 |
| Mg | 0,80 | 0,20 | 1,20 | 1,48 | 0,00 | 0,00 | 0,00 |
| Ca | 0,12 | 0,00 | 0,00 | 0,00 | 0,36 | 0,00 | 0,02 |
| Na | 0,00 | 0,00 | 0,00 | 0,01 | 0,60 | 0,14 | 0,05 |
| K | 0,00 | 0,00 | 0,00 | 0,82 | 0,01 | 0,86 | 0,51 |
| H | 0,00 | 0,00 | 0,50 | 2,00 | 0,00 | 0,00 | 0,42 |
| $X_{Fe}$ | 0,71 | 0,80 | 0,39 | 0,69 | | | |
| Vol % | 28,0 | 13,0 | 18,0 | 1,0 | 10,0 | 5,0 | 15,0 |
| (includes 10% sillimanite, 5 % ilmenite) | | | | | | | |

calculated phase compositions and volume proportions at $830 \pm 50°C$, $5.8 \pm 0.5$ kbar

| | Garnet | Spinel | Cordierite | Biotite | Plagioclase | K-feldspar | Melt |
|---|---|---|---|---|---|---|---|
| Si | 3,00 | 0,00 | 5,00 | - | 2,00 | - | 3,24 |
| Ti | 0,00 | 0,00 | 0,00 | - | 0,00 | - | 0,00 |
| Al | 2,00 | 2,00 | 4,00 | - | 1,00 | - | 0,78 |
| Fe | 1,87 | 0,71 | 0,60 | - | 0,00 | - | 0,03 |
| Mg | 0,91 | 0,29 | 1,40 | - | 0,00 | - | 0,01 |
| Ca | 0,19 | 0,00 | 0,00 | - | 1,00 | - | 0,02 |
| Na | 0,00 | 0,00 | 0,00 | - | 0,00 | - | 0,22 |
| K | 0,00 | 0,00 | 0,00 | - | 0,00 | - | 0,36 |
| H | 0,00 | 0,00 | 0,48 | - | 0,00 | - | 1,55 |
| $X_{Fe}$ | 0,67 | 0,71 | 0,30 | - | | | |
| Vol % | 35,0 | 4,0 | 27,0 | - | 2,0 | - | 28,0 |
| (includes 3 % sillimanite, 1 % ilmenite) | | | | | | | |

Note: Best match as determined by $X_{Fe}$ nearness of Grt, Spl and Crd, and from ratios of product phases in corona.

Chemical compositions of minerals were obtained by using wavelength-dispersive spectrometry and back-scattered electron images on a JEOLJXA-8200 Superprobe electron probe micro-analyzer (EPMA) at Massachusetts Institute of Technology (MIT), Cambridge, USA. The silicate phases were analyzed at MIT using an accelerating voltage of 15 kV, a beam current of 10 nA, and 40–60 s counting times per element. Typical $1\sigma$ standard deviation of counts was between 0.5 and 1%. The beam diameter was generally focused to ∼ 1 μm for solid phases, but was defocused to ∼ 5–10 μm for glass analysis.