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Life cycle analysis of coesite-bearing garnet by Jan Schönig, Hilmar von Eynatten, Guido Meinhold, and N. Keno Lünsdorf

Supplementary Material 3:

Details of step-wise garnet classification

To assign the individual coesite-bearing garnet grains to their most likely source, i.e. felsic or mafic, a step-wise classification is performed by comparing their chemistry and mineral inclusion assemblage with that of garnet from crystalline rocks in the catchment areas. In the first four steps, the molar proportions of X_{Ca}, X_{Fe}, and X_{Mg} are considered (Fig. 7). For step I, it seems reasonable to assume that garnet grains matching with the 50 % confidence ellipsoid of diamond-bearing paragneiss are of felsic origin, whereas those matching with the 50 % confidence ellipsoid of eclogite are derived from mafic rocks. By this means, 21 out of the 93 coesite-bearing grains are assigned to their source. For step II, the boxplot of the X_{Ca} component in terms of the local crystalline rocks shows that all garnet from eclogite contains $X_{Ca} \geq 0.186$. Thus, all coesite-bearing garnet grains with a lower amount of the X_{Ca} component can be assigned to a felsic source (45 out of the 72 remaining unclassified coesite-bearing grains after step I). With regard to the X_{Fe} component, garnet of local eclogite has values ≤ 0.585 and felsic rocks show values ≥ 0.449. Based on these limits, in step III, all coesite-bearing garnet grains with $X_{Fe} > 0.585$ are assigned to a felsic source and grains with $X_{Fe} < 0.449$ to a mafic source, leading to an assignment of 5 out of the 27 remaining after step II. One additional coesite-bearing garnet can be assigned to a felsic source in step IV based on the low X_{Mg} component, which is ≥ 0.180 for garnet of local eclogite. In summary, after step IV, 72 out of the 93 coesite-bearing garnet grains (~77 %) are assigned to their most likely source, whereby one quarter belongs to a mafic and three quarters belong to a felsic source.

The 21 remaining coesite-bearing garnet grains after step IV are more difficult to assign as they show strong overlap with compositions of garnet from both country rock gneiss and eclogite. To tackle this issue, at first, a principal component analysis was performed on the, so far, unassigned grains. For that, all measured oxide weight percentages were used, except Cr_2O_3 due to amounts that are exclusively below the detection limit. Prior analysis, the data was centered log-ratio transformed. Based on the biplot, the log ratios of the variables FeO/(CaO+MgO) and CaO/MgO are most suitable for further analysis (Fig. SM3a).

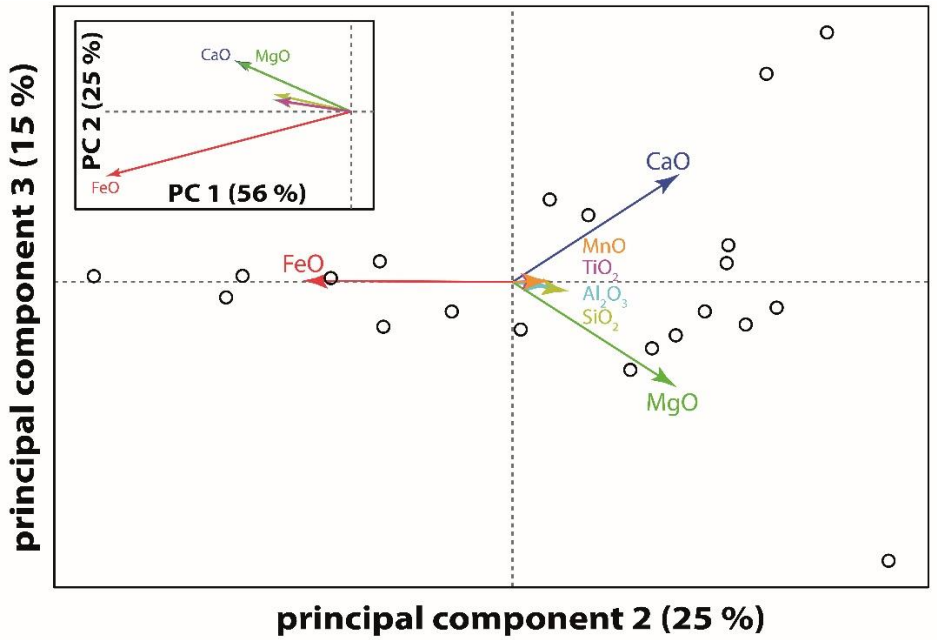

Figure SM3a: Biplot showing principal components two and three of the centered log-ratio transformed compositional data of the unassigned coesite-bearing garnet grains after classification step IV. Inset shows principal components one and two.

For step V, the composition of the coesite-bearing garnet grains is shown in a scatter plot using the afore-mentioned ratios in comparison to mineral inclusion assemblages co-existing with coesite (Fig. 8). As discussed in Section 4.b., inclusions of omphacite are characteristic of an eclogitic source. This is again supported by omphacite inclusions occurring together with coesite in two out of the 18 garnet grains assigned to a mafic source in the steps before, and the absence of omphacite inclusions in all coesite-bearing grains assigned to a felsic source. Thus, three of the unclassified

grains containing coesite co-existing with omphacite and overlapping with the 95 % confidence ellipsoid of local eclogite can be confidently assigned to a mafic source. In contrast, garnet containing graphite inclusions point to a felsic source, which is again supported by their occurrence in 13 out of the 54 coesite-bearing garnet grains previously assigned to a felsic source, and their absence in mafic coesite-bearing garnet. In addition, inclusions of alkali feldspar, phlogopite–biotite, and cristobalite solely occur in coesite-bearing garnet assigned to a felsic source, and quartz inclusions dominantly occur in felsic garnet. These inclusion types furthermore often form mineral assemblages in the coesite-bearing detrital garnet grains of felsic affinity. Thus, considering these inclusion types, seven of the hitherto unclassified grains can be assigned to a felsic source (Fig. 8).

From the remaining 11 not-assigned coesite-bearing grains after step V, five show a compositional contrast to local eclogite and compositions similar to garnet previously assigned to a felsic source (Fig. 8). These five grains are assigned to a felsic source in step VI, ending up with a total of 87 out of the 93 coesite-bearing garnet grains (~94 %) assigned to their most likely source. From these 87 grains, 66 (~76 %) were assigned to a felsic and 21 (~24 %) to a mafic source. Their frequency and grain-size relations for the seven sediment samples are shown in Figure 9. For some of the remaining six coesite-bearing grains unassigned after step VI, there are subordinate indications for belonging to a felsic origin like inclusions of apatite and kyanite, which often occur in the coesite-bearing felsic grains (Fig. SM3b). However, both inclusion types are also present in some of the mafic grains, and compositionally they do not clearly favor a felsic or mafic source. In either case, assigning all of the six remaining garnet grains to a felsic or a mafic source, changes in the grain-size pattern of coesite-bearing garnet are negligible (cf. Figs. 9 and SM3c). We thus use the ~94 % of coesite-bearing garnet grains confidently assigned in steps I–VI for further discussion.

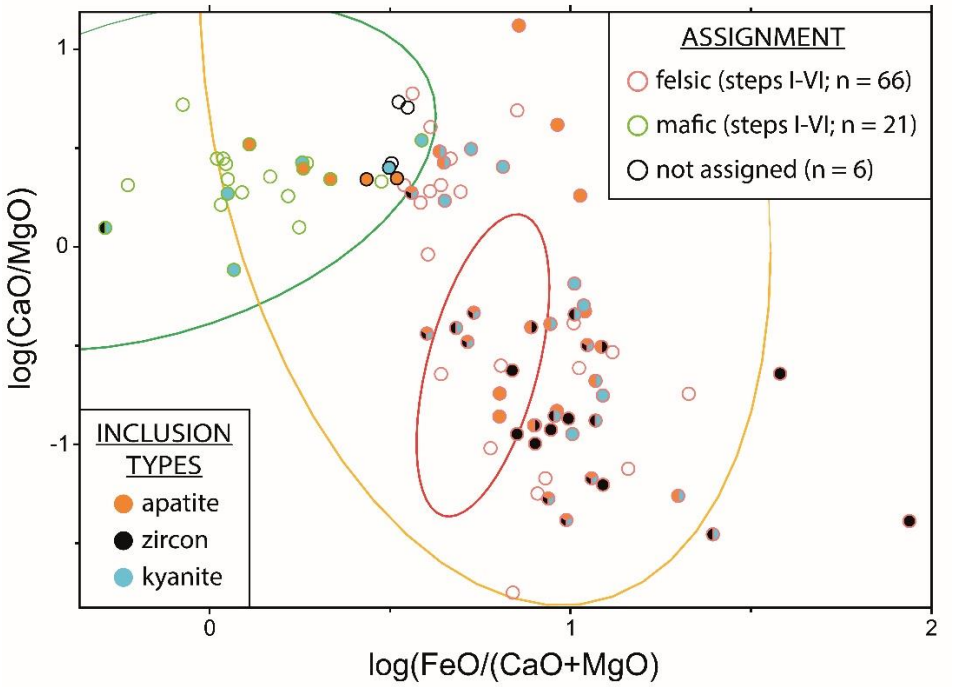

Figure SM3b: Assignment of coesite-bearing garnet to their most likely source after step VI based on log-ratio plots in comparison with mineral inclusion assemblages. Log-ratios are chosen based on the principal component analysis biplot shown in Figure C1. For comparison, garnet composition of local crystalline rocks compiled by Schönig *et al.* (2020) are shown as 95 % confidence ellipsoids with colors similar to Fig. 7.

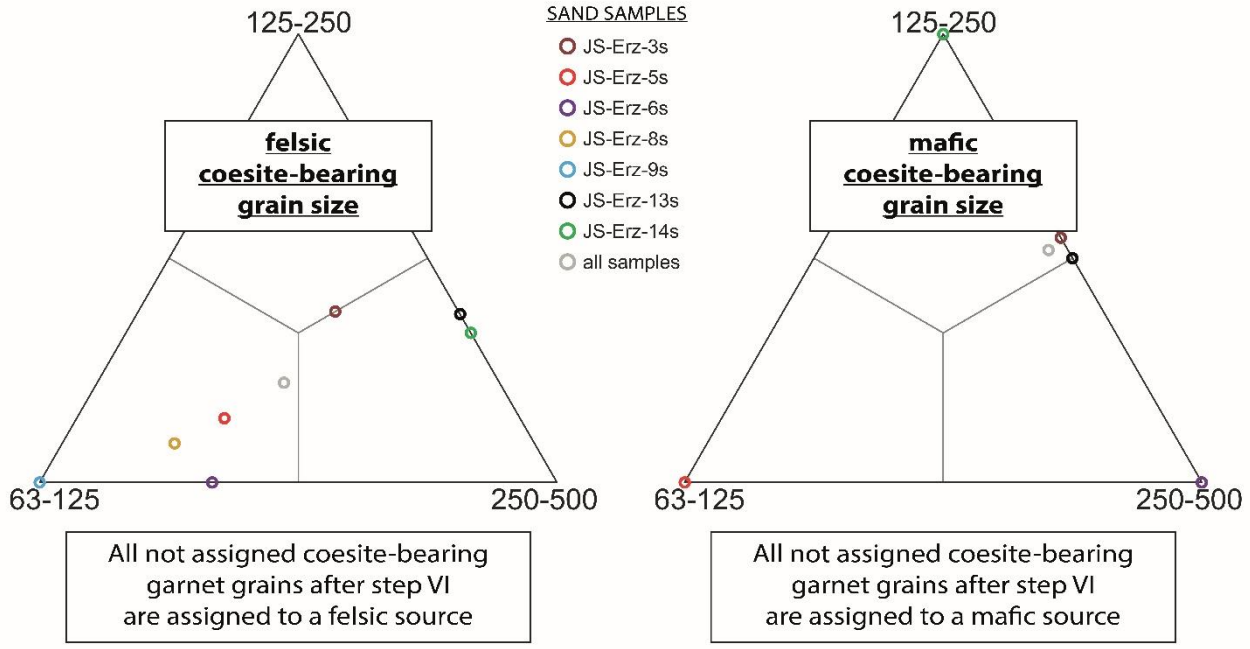

Figure SM3c: Theoretical grain-size distribution of felsic and mafic coesite-bearing garnet grains if all unassigned grains after step VI are assigned to a felsic or mafic source, respectively.