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Diamond and coesite inclusions in detrital garnet of the Saxonian Erzgebirge, Germany

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DATA REPOSITORY 1: SAMPLES & METHODS

Samples

Coordinates of the seven investigated modern sand samples marked in Figure 1 are given in Table DR1.

Modern sands were wet sieved to extract the 125–250 μm grain-size fraction, treated with acetic acid, and the heavy mineral fraction was separated by centrifugation using sodium polytungstate with a density of 2.83–2.88 g cm^{-3} and embedded in synthetic mounts using a bonding epoxy. The mounts were grounded with silicon carbide abrasive paper and polished in five steps with Al_2O_3 abrasives in water suspension up to the finest step with a particle size of 0.05 μm .

TABLE DR1. COORDINATES OF MODERN SAND SAMPLING LOCATIONS

Sample	Northing	Easting	Creek/River width	Type
JS-Erz-3s	50.74352°	13.24847°	~1.5 m	mixed sample (~5 m sector)
JS-Erz-5s	50.73924°	13.26169°	~3.0 m	mixed sample (~10 m sector)
JS-Erz-6s	50.73537°	13.29782°	~1.0 m	mixed sample (~20 m sector)
JS-Erz-8s	50.74233°	13.30458°	~1.0 m	mixed sample (~10 m sector)
JS-Erz-9s	50.72633°	13.25883°	~1.5 m	mixed sample (~10 m sector)
JS-Erz-13s	50.74862°	13.19472°	~4.0 m	mixed sample (~10 m sector)
JS-Erz-14s	50.76142°	13.17091°	~20.0 m	mixed sample (~60 m sector)

Raman spectroscopy

From each of the seven samples, all mineral inclusions $\geq 2 \mu\text{m}$ were identified in 100 detrital garnets (those without mineral inclusions $\geq 2 \mu\text{m}$ were not taken into account) by using a Horiba Jobin Yvon XploRA Plus Raman spectrometer equipped with an Olympus BX41 microscope at the University of Göttingen (Geosciences Center, Department of Sedimentology and Environmental Geology). The obtained inclusion spectra were compared with the RRUFF database (Lafuente et al., 2015). Measurements were performed using a 532 nm laser ($\sim 11 \text{ mW}$ at sample surface), a 1800 l mm^{-1} grating, an $100\times$ LWD objective with a numerical aperture of 0.8, and a confocal hole diameter and slit of $100 \mu\text{m}$. The spectrometer was calibrated on the 520.7 cm^{-1} line of silicon, and the recorded spectrum was centered at 840 cm^{-1} , covering a spectral field between $\sim 70 \text{ cm}^{-1}$ and $\sim 1650 \text{ cm}^{-1}$. The method of inclusion identification and the classification of inclusion types are described in Schönig et al. 2018b. In this study, we did not discriminate between apatite and monazite due to their similar Raman spectra and the limited significance for source rock characterization. However, randomly we checked the OH-region between 3000 and 4000 cm^{-1} of the inclusion spectra and note the presence or absence of OH under remarks in Table DR2.

To determine the position of the main bands of diamond and coesite inclusions, the Raman spectra of all identified inclusions were captured again using a specific calibration and correction method. The 2400 l mm^{-1} grating was used to achieve the highest resolution. For diamond inclusions the spectrometer was calibrated on the 1331.7 cm^{-1} line of diamond, and for coesite inclusions on the 520.7 cm^{-1} line of silicon. The center of the spectrum was left in the same position like during the calibration, i.e., 1331.74 cm^{-1} and 520.62 cm^{-1} , respectively. These positions are close to the positions of the diamond ($\sim 1331.7 \text{ cm}^{-1}$) and coesite ($\sim 520.7 \text{ cm}^{-1}$) main bands at atmospheric pressure and room temperature (e.g., Krishnamurti, 1954; Schönig et al., 2018a). Due to possible small inaccuracies of the calibration, a possible drift during the measurement sessions and/or a possible stretching or compression of the spectral field, a correction of the main band positions was performed using distinctive spectral lines of a neon glow lamp as reference positions. The light of the neon glow lamp was captured simultaneously with the spectrum from every inclusion by using a laser power of $\sim 0.04\text{--}4.44 \text{ mW}$ and an acquisition time of $600\text{--}1200 \text{ s}$. Spectra evaluation was performed within the Labspec 6.4.4 software by subtracting the background by a polynomial baseline fit, adding Gaussian Lorentzian mixed functions (pseudo-Voigt) at up to four selected neon reference line positions and the diamond/coesite main band, and fitting the functions to the captured spectra. Selected neon reference line positions are Ne #1 at 568.982 nm (i.e., 1214.667 cm^{-1}

relative), Ne #2 at 571.923 nm (i.e., 1305.044 cm^{-1} relative), Ne #3 at 574.830 nm (i.e., 1393.475 cm^{-1} relative), and Ne #4 at 576.442 nm (i.e., 1442.126 cm^{-1} relative) for diamond; and Ne #1 at 540.065 nm (i.e., 273.336 cm^{-1} relative), Ne #2 at 541.265 nm (i.e., 314.684 cm^{-1} relative), Ne #3 at 543.365 nm (i.e., 386.093 cm^{-1} relative), and Ne #4 556.277 nm (i.e., 813.263 cm^{-1} relative) for coesite. The measured main band position of every diamond/coesite was corrected by a quadratic regression function (linear when only two neon lines are considered) based on the difference between the measured neon line positions compared to their reference positions. Based on the determined diamond main band positions compared to the positions at atmospheric pressure and room temperature, inclusion pressures were calculated by using the experimentally ratio of 1 GPa per 2.64 cm^{-1} for diamond (Tardieu et al., 1990). Results are given in Tables DR3 and DR4.

Inclusion sizes were determined within the Labspec software using the 100 \times LWD objective. Stated are the long and short axes (0.5 μm steps) in a two dimensional (plane) view as situated in the garnet grains and embedded in the epoxy. The closest distance to the garnet surface was determined by focusing through the grain, which can be slightly imprecise if the closest distance is in direction of the lower surface.

Electron microprobe

After inclusion analysis by Raman spectroscopy, the chemical composition of all analyzed garnets that contain inclusions $\geq 2 \mu\text{m}$ was determined by wavelength-dispersive spectroscopy (Table DR5). Measurements were performed at the University of Göttingen (Geosciences Center, Department of Geochemistry) using a JEOL JXA 8900 RL electron microprobe equipped with five wavelength dispersive spectrometers. Before analysis, all samples were coated with carbon to ensure conductivity. Measurement conditions include an accelerating voltage of 15 kV and a beam current of 20 nA. Counting times were 15 s for Si, Mg, Ca, Fe and Al, and 30 s for Ti, Cr and Mn. The spot of the electron beam was adjusted to the center of the garnet grains except for grains with fractures or inclusions at the center, where the beam spot was adjusted to an undisturbed garnet mantle position. From the 700 analyzed garnets, four measurement results were discarded (totals not close to 100 wt% or interference with inclusions). The composition of diamond- and coesite-bearing garnets was determined at nine spots of each garnet: one at the center, four at the mantle, and four at the rim (in each case two in horizontal (x) direction and two in vertical (y) direction). For garnet classification, besides the molar proportions plotted in Fig. 3, also multivariate statistics after Tolosana-

Delgado et al. (2018) were performed using the prior probability ‘equal-M’ (Fig. DR1). The results support the trends observed in the Fig. 3.

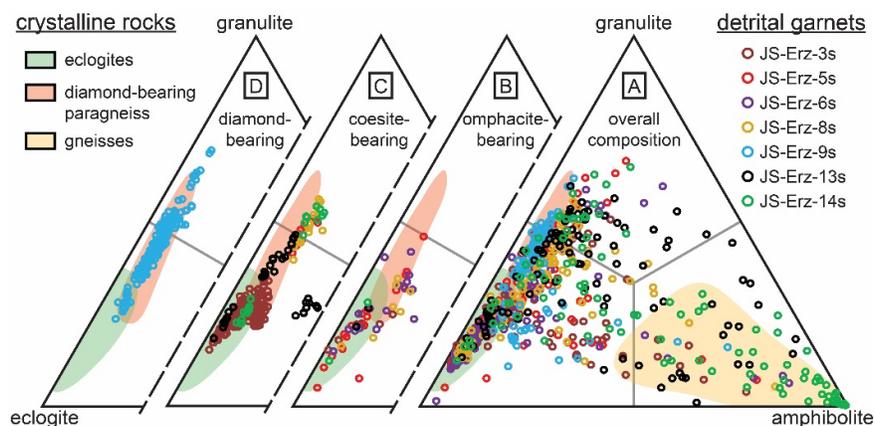


Figure DR1: Geochemical classification of detrital garnets in after Tolosana-Delgado et al. (2018) showing the probabilities of being derived from eclogite-, granulite-, or amphibolite-facies rocks. The entire EMPA dataset is given in Table DR5. A: Probabilities of all detrital garnets (n = 696; one spot per grain). B: Probabilities of omphacite-bearing garnets (n = 51; one spot per grain; one outlier not shown). C: Probabilities of coesite-bearing garnets (n = 234; 9 spots per grain). D: Probabilities of diamond-bearing garnets (n = 198; 9 spots per grain). For comparison, garnet data of local crystalline rocks are shown as envelopes (Table DR6).

ADDITIONAL DATA REPOSITORY TABLES (EXCEL FILES)

TABLE DR2. MINERAL INCLUSION DATA

TABLE DR3. COESITE INCLUSIONS

TABLE DR4. DIAMOND INCLUSIONS

TABLE DR5. EMPA OF DETRITAL GARNETS

TABLE DR6. GARNET CHEMISTRY OF LOCAL CRYSTALLINE ROCKS

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