

# **HOW GEOMETRY AND ANISOTROPY AFFECT RESIDUAL STRAIN IN HOST-INCLUSION SYSTEM: COUPLING EXPERIMENTAL AND NUMERICAL APPROACHES**

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## **SUPPLEMENTARY MATERIAL**

### **S.1 SAMPLE PROVENANCE AND GEOLOGICAL BACKGROUND: THE DORA MAIRA MASSIF**

Our study focusses on solid inclusions in pyrope megablasts (up to 15 cm across) and porphyroblasts (up to 2 cm across) from the Dora Maira Massif (DMM; Italian Western Alps; Fig. DR1), a slice of continental crust involved in Alpine subduction and exhumation. Since the discovery of coesite inclusions in garnet from phengite white-schists (Chopin, 1984), the DMM became a world-known setting for ultrahigh-pressure (UHP) metamorphism and attracted interest of numerous scientists who defined its structure, tectonic and metamorphic histories (e.g. Chopin, 1984; Hermann, 2003). The DMM consists of Variscan orto- and para-gneiss involved in Alpine subduction and exhumation (for a review see also Carswell and Compagnoni, 2005). The UHP, coesite-bearing Brossasco-Isasca Unit of the DMM is tectonically sandwiched between two lower pressure units (Rocca du Soleil and Pinerolo Units, Fig. S.1). It consists of two main lithostratigraphic sub-units, the Monometamorphic and the Polymetamorphic Complexes, made of orthogneiss and of amphibolite-facies basement rocks, respectively. We investigated pyrope megablasts and porphyroblasts from whiteschist lenses hosted in the Monometamorphic Complex (Gilba locality, Fig. S.1). The whiteschist is interpreted to either derive from evaporite (Chopin, 1984), or from metasomatism of

former orthogneiss by Mg-rich fluids infiltrating during UHP metamorphism (e.g. Ferrando et al., 2009);. The P-T-t path of the DMM has been defined in a number of papers: here we refer to Rubatto and Hermann, (2001), who combined P-T estimates with in-situ U-Pb titanite dating. These authors defined a peak metamorphic stage at 3.5 GPa - 750°C at  $35.1 \pm 0.9$  Ma, and three decompression steps at  $32.9 \pm 0.9$  Ma,  $31.8 \pm 06$  Ma and  $29.9 \pm 1.4$  Ma, respectively. Rubatto & Hermann (2001) proposed different exhumation velocities of the DMM, from 3.4 cm/yr during the first stage of exhumation from peak conditions, to 1.6 cm/yr and 0.5 cm/yr during the last two exhumation steps. More recently, further experimental and petrological studies carried out on whiteschists by Hermann (2003) indicated that the peak metamorphic pressure was in the diamond facies stability field at 43 kbar and 730 °C.

## **S.2 MINERAL CHEMISTRY OF GARNET AND ZIRCON**

The mineral chemistry of garnets was determined by means of a TESCAN Vega-3 electron microprobe at the University of Genova (DISTAV department), using an energy-dispersive technique with an acceleration voltage of 15 keV, a beam current of 14 nA. The standard used were: K pyrope USNM 143968, MAC N° 10642 forsterite. Empirical formula recalculation was computed based on 12 oxygens and the ferric iron was estimated by filling octahedral sites to the theoretical value of 2.0 per formula unit (see Table S.1). The electron microprobe analysis and chemical element mapping of the idiomorphic polished zircon was performed using a Cameca SX-100 SEM system electron microprobe available at University of Hamburg (Earth Science department), using a wavelength-dispersive technique with an acceleration voltage of 15 keV, a beam current of 40 nA. The standard used were: Al<sub>2</sub>O<sub>3</sub> for Al, ZrSiO<sub>4</sub> for Si and Zr, apatite for P, wollastonite for Ca, MnTiO<sub>3</sub> for Mn, andradite for Fe, REE1 for Y, REE2 for Ce, REE4 for Nd, Hf for Hf, Pb-Glas for Pb, Th-Glas for Th, UO<sub>2</sub> for U. Where REE1 = Si : 23.27%, Al : 6.23%, Ca : 13.43%, Y : 3.97%, Pr : 3.93%, Dy : 4.02%, Er : 3.97%, O : 40.46%, REE2 = Si : 23.53%, Al : 6.3%, Ca : 13.49%, Ce : 3.93%, Eu : 3.99%, Ho : 3.92%, Tm : 4.01%, O : 40.47% and REE4 = Si : 24.76%, Al : 6.66%, Ca : 14.42%, Nd : 3.89%, Tb

: 4.%, Lu : 3.97%, O : 41.8%. Empirical formula recalculation was computed on the basis of 16 oxygens per formula unit.

Garnets, with colors ranging from pale to dark pink, occur either as megablasts (up to 15 cm across) and porphyroblasts (up to 1 cm across) in coesite-bearing whiteschists from the Brossasco-Isasca UHP unit. The garnet megablast (sample DMG.2), in which the selected polished zircon inclusions have been studied, displays a pyrope-rich composition (up to 94 mol%) with minor amounts of almandine (up to 5 mol%) and grossular (< 2 mol%) from the core to the rim. Garnet porphyroblasts display a zonation characterized by almandine-rich (up to 20 mol%) cores and almost pure pyrope rims (up to 95 mol%) (see Figure S.2). The variation of Mg and Fe components in garnet is antipathetic whereas the grossular component seldom reaches 3 mol%. The most outer garnet rims often show an increase in the almandine component that was already interpreted by previous authors as the result of retrogression in the later metamorphic stages. Table 1 reports some representative chemical analysis of both the garnet megablasts and porphyroblasts.

We performed chemical analysis on the idiomorphic elongated crystal of zircon in order to understand if the heterogeneity in Raman peak position was caused by the presence of heterogeneity in the chemical composition (i.e. zonation). It is important to stress that Raman peak positions are commonly influenced by chemical variation greater than 1 wt % and therefore WDS microprobe analysis are sufficient for our purposes. Chemical analyses performed on the same points in which Raman spectra were collected show no significant chemical heterogeneities for this zircon crystal. Zircon chemical analyses results are reported in Table S.1.

### **S.3 SELECTION RULES FOR PHONON MODES IN ZIRCON AND COESITE, AND DATA ACQUISITION AND EVALUATION**

Zircon has tetragonal symmetry with space group  $I4_1/amd$ . According to group theory analysis, the optic phonons at the Brillouin-zone center of zircon are (Kroumova et al., 2003):

$$\Gamma_{opt} = 2A_{1g} + A_{1u} + A_{2g} + 3A_{2u} + 4B_{1g} + B_{1u} + B_{2g} + 2B_{2u} + 5E_g + 4E_u$$

The  $A_{1g}$ ,  $B_{1g}$ ,  $B_{2g}$  and  $E_g$  modes are Raman-active and therefore a total of 12 Raman peaks can be observed in the spectrum of a randomly oriented zircon.

According to previous experimental results (Knittle and Williams, 1993; Mihailova et al. unpublished data) the  $B_{1g}$  mode near  $1008\text{ cm}^{-1}$ , the  $A_{1g}$  mode near  $975\text{ cm}^{-1}$  and the  $E_g$  mode near  $357\text{ cm}^{-1}$  are the most pressure-sensitive peaks. For this reason, our discussion is mainly focused on these vibrational modes. Note that the  $B_{1g}$  modes are symmetry allowed in  $\bar{y}(xx)y$  scattering geometry (Porto's notation),  $A_{1g}$  in  $\bar{y}(xx)y$ ,  $\bar{y}(zz)y$ , and  $\bar{z}(xx)z$ , whereas  $E_g$  in  $\bar{y}(xz)y$ , with  $x$ ,  $y$ ,  $z$  along the  $a$ ,  $b$  and  $c$  crystallographic axes, respectively.

Coesite is a monoclinic crystal with space group  $C2/c$  (unique axis  $b$ ). The irreducible representation of the optical vibrations are (Kroumova et al., 2003):

$$\Gamma_{opt} = 16A_g + 18A_u + 17B_g + 18B_u$$

The  $A_g$  and  $B_g$  modes are Raman-active and therefore a total of 33 Raman peaks can be theoretically observed in the spectrum of a randomly oriented coesite crystal.

Experimental results by Hemley (1987) suggest that the  $A_g$  mode near  $119\text{ cm}^{-1}$ , near  $183\text{ cm}^{-1}$  and near  $521\text{ cm}^{-1}$  are the most pressure-sensitive Raman peaks and they were used as our "sensors" for the polishing effect in coesite. However not all of the peaks predicted by group theory were observed in our spectra because of their weak intensities or because of partial overlap with the main garnet peaks.

Micro-Raman scattering measurements were conducted in backscattering geometry with a Horiba Jobin-Yvon T64000 triple-monochromator spectrometer (holographic gratings of 1800 grooves/mm) equipped with an Olympus BX41 confocal microscope (Olympus LM Plan FLN 50 $\times$  objective with a numerical aperture of 0.5) and a Symphony liquid-N<sub>2</sub>-cooled charge-coupled device detector. Raman spectra were excited either by the 488.0 or 514.532 nm line of a Coherent 90C Fred Ar<sup>+</sup> laser, in order to achieve a minimum level of continuum photoluminescence background. For both laser lines the laser power on the sample surface was approximately 14 mW, to avoid sample overheating during the experiment. The spectrometer was calibrated to the silicon Raman peak at  $520.5\text{ cm}^{-1}$ . The

spectral resolution was  $\sim 2 \text{ cm}^{-1}$  and the instrumental accuracy in determining the peak positions was  $\sim 0.35 \text{ cm}^{-1}$ . Parallel and cross polarized Raman spectra were collected for all samples in the spectral range 15–1215  $\text{cm}^{-1}$ . In the case of zircon S3, the grains were oriented with the *c* axis perpendicular to the polarization of the incident light, which ensured maximum Raman intensity of the major peak near 1008  $\text{cm}^{-1}$ . Spectra were collected for 7 s averaging over 3 accumulations. For each inclusion a series of spot measurements were carried out along the equatorial plane of the inclusion as shown in Figure 3. OriginLab-Pro 2018 software package was used for data fitting and evaluation. The collected spectra were baseline corrected for the continuum luminescence background when necessary, temperature-reduced to account for the Bose-Einstein occupation factor (Kuzmany, 2009) and normalized to the acquisition time. Peak positions, full-widths at half maximum (FWHMs), and integrated intensities were determined from fits with pseudo-Voigt functions [PV = (1 – q)·Lorentz + q·Gauss, q is the weight coefficient]. The criterion for the maximum number of fitted peaks was  $\Delta I < I/2$ , where *I* and  $\Delta I$  are the calculated magnitude and uncertainty of each peak intensity, respectively.

#### **S.4 FINITE ELEMENT (FE): COMPUTATIONAL DETAILS**

We have used a commercially available engineering package, Abaqus Standard v.2016 (Dassault Systèmes, Simulia, Providence), to create and analyze 3D finite-element models following the same procedures outlined in Mazzucchelli et al., 2018. The models reproduce the geometry and the crystallographic orientations of our zircon inclusions in pyrope (samples S2 and S3), at several steps of distance of the inclusion from the external surface of the host.

All our 3D models have at least one mirror plane, therefore only half of the selected shape was created and the full model was obtained by reflection through that mirror plane. Since the mirror plane of the model corresponds to the [1 0 0] crystallographic plane, it does not restrict the deformation of zircon that is tetragonal. The resulting model consisted of more than 400000 10-node quadratic tetrahedral elements (element C3D10 in the Abaqus library). Material properties and boundary conditions were assigned, and then a mesh convergence analysis was performed. The mesh was refined in the areas

with higher stress gradients until the calculated stress distribution appeared smooth. An example of one model and the mesh used is reported in Fig. S.3. To simulate the external pressure, face loads were applied to the 3D elements on the external boundaries of the host. Boundary conditions were placed on the appropriate edges and faces of the models to avoid rigid body rotation and translation in the x, y and z directions.

The constitutive equation used by Abaqus for anisotropic linear elasticity is:

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl}$$

where  $\sigma_{ij}$  and  $\epsilon_{kl}$  are the stress and the strain tensor respectively, and  $C_{ijkl}$  are the elastic stiffness moduli. For the zircon inclusion the elastic stiffness moduli at room conditions reported by Ozkan et al. (1974) were used in FE analysis (Table DR.7). The pyrope host was treated as isotropic because its universal anisotropic index (Ranganathan and Ostoja-Starzewski, 2008) is only  $9 \times 10^{-4}$ , essentially zero, based on the elastic moduli reported by Sinogeikin and Bass (2002). The isothermal bulk modulus at room conditions was derived from Milani et al. (2015) while the shear modulus was obtained from the elastic moduli reported by Sinogeikin and Bass (2002).

## S.5 RESIDUAL PRESSURE ESTIMATION

Residual “pressure” estimation from Raman shift frequencies made using the approach given by Murri et al., (2018) is reported in table S.8. The phonon frequencies taken as reference for the  $B_{1g}$  and the  $A_{1g}$  modes refer to the zircon crystal S3 once completely exposed to the external surface of the host ( $1008.68 \text{ cm}^{-1}$  and  $974.85 \text{ cm}^{-1}$ ). Note that these reference values are in agreement with free zircon crystals having similar composition (Binvignat et al., 2018).

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TABLE S.1. REPRESENTATIVE CHEMICAL ANALYSIS OF ZIRCON SAMPLE S3 AND GARNET MEGABLASTS AND PORPHYROBLASTS FROM WHITESCHISTS

Zircon							mineral				
Mineral	American Mineralogist: December 2018 Deposit AM-18-126700						mineral	garnet megablast		garnet porphyroblasts	
p. analysis	p1	p2	p3	p4	p5	p6	p. analysis	core	rim	core	rim
oxide	(wt%)	(wt%)	(wt%)	(wt%)	(wt%)	(wt%)	oxide	(wt%)	(wt%)	(wt%)	(wt%)
Al <sub>2</sub> O <sub>3</sub>	0.01	0.00	0.00	0.00	0.00	0.01	SiO <sub>2</sub>	42.50	42.85	42.14	42.83
SiO <sub>2</sub>	32.85	32.42	32.74	32.50	32.40	31.60	TiO <sub>2</sub>	b.d.l.	b.d.l.	0.16	0.00
P <sub>2</sub> O <sub>5</sub>	0.23	0.40	0.27	0.27	0.35	0.09	Al <sub>2</sub> O <sub>3</sub>	25.11	25.00	24.64	25.23
CaO	0.02	0.02	0.01	0.02	0.02	0.02	Cr <sub>2</sub> O <sub>3</sub>	b.d.l.	b.d.l.	b.d.l.	b.d.l.
MnO	0.01	0.02	0.01	b.d.l.	0.01	b.d.l.	Na <sub>2</sub> O	b.d.l.	b.d.l.	b.d.l.	b.d.l.
Fe <sub>2</sub> O <sub>3</sub>	0.10	0.17	0.12	0.14	0.11	0.20	FeO	2.80	3.36	8.98	2.82
Y <sub>2</sub> O <sub>3</sub>	b.d.l.	0.00	b.d.l.	b.d.l.	b.d.l.	b.d.l.	MgO	28.16	28.13	23.04	28.30
ZrO <sub>2</sub>	66.11	64.04	65.44	64.55	65.17	66.51	MnO	b.d.l.	b.d.l.	b.d.l.	0.09
Ce <sub>2</sub> O <sub>3</sub>	b.d.l.	b.d.l.	0.01	b.d.l.	b.d.l.	b.d.l.	CaO	0.86	0.73	1.31	0.93
HfO <sub>2</sub>	1.49	1.64	1.45	1.43	1.52	1.69	H <sub>2</sub> O+	b.d.l.	b.d.l.	b.d.l.	b.d.l.
PbO	b.d.l.	b.d.l.	b.d.l.	0.03	0.01	b.d.l.	H <sub>2</sub> O-	b.d.l.	b.d.l.	b.d.l.	b.d.l.
ThO <sub>2</sub>	0.02	b.d.l.	b.d.l.	0.03	b.d.l.	b.d.l.	Sum	99.43	100.07	100.27	100.20
UO <sub>2</sub>	0.07	0.14	0.03	0.09	0.07	0.04					
Nd <sub>2</sub> O <sub>3</sub>	b.d.l.	0.02	0.03	b.d.l.	0.01	0.03					
Sum	100.91	98.87	100.10	99.07	99.68	100.19					
Occupancy	moles	moles	moles	moles	moles	moles	occupancy	moles	moles	moles	moles
Zr	3.92	3.86	3.90	3.89	3.91	4.01	Si	2.92	2.93	2.95	2.92
Hf	0.05	0.06	0.05	0.05	0.05	0.06	Al	0.08	0.07	0.05	0.08
U	-	0.01	-	-	-	-	Sum site IV	3.00	3.00	3.00	3.00
Th	-	-	-	-	-	-	Al	1.95	1.95	1.99	1.95
Y	-	-	-	-	-	-	Fe <sup>3+</sup>	0.05	0.05	0.01	0.05
Al	-	-	-	-	-	-	Cr <sup>3+</sup>	-	-	-	-
Ca	-	-	-	-	-	-	Sum site VI	2.00	2.00	2.00	2.00
Mn	-	-	-	-	-	-	Fe <sup>2+</sup>	0.11	0.14	0.51	0.11
Fe <sup>3+</sup>	0.01	0.02	0.01	0.01	0.01	0.02	Mg	2.88	2.87	2.41	2.88
Sum VIII site	3.98	3.94	3.97	3.96	3.98	4.09	Mn <sup>2+</sup>	-	-	-	0.01
P	0.02	0.04	0.03	0.03	0.04	0.01	Ca	0.06	0.05	0.10	0.07
Si	3.99	4.01	4.00	4.01	3.98	3.90	Na <sub>2</sub> O	-	-	-	-
Sum IV site	4.01	4.05	4.03	4.04	4.02	3.91	Sum site VIII	3.06	3.06	3.01	3.06

TABLE S.2: RAMAN SHIFT HETEROGENEITY INSIDE ONE SINGLE CRYSTAL

p. analysis*	B <sub>1g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	A <sub>1g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	E <sub>g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )
p6	1011.90(1)	5.30(2)	978.51(8)	4.84(12)	360.07(1)	7.44(8)
p5	1012.09(2)	5.61(3)	977.66(9)	5.35(16)	358.90(2)	8.07(9)
p4	1011.60(2)	6.02(3)	977.56(9)	5.34(16)	358.77(2)	7.82(9)
p3	1011.18(2)	6.18(3)	978.10(7)	5.28(12)	359.65(2)	7.30(7)
p2	1011.26(2)	6.31(5)	978.41(7)	5.15(12)	359.98(2)	7.51(6)
p1	1012.18(2)	5.72(4)	978.34(7)	4.79(11)	360.08(2)	6.94(6)
p. analysis†	B <sub>1g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	A <sub>1g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	E <sub>g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )
p6	1010.03(1)	5.71(3)	976.23(5)	4.86(8)	358.37(1)	7.50(2)
p5	1010.05(2)	6.38(3)	976.30(5)	5.50(8)	358.25(1)	7.77(3)
p4	1009.37(2)	5.86(3)	975.60(5)	4.97(9)	357.51(1)	7.36(2)
p3	1009.05(2)	6.63(4)	975.32(8)	5.39(16)	357.13(1)	8.08(3)
p2	1008.99(2)	6.23(4)	975.37(8)	5.23(15)	357.17(1)	7.68(4)
p1	1009.92(2)	5.92(4)	976.18(9)	4.77(14)	357.96(1)	6.78(4)
p. analysis§	B <sub>1g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	A <sub>1g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	E <sub>g</sub> (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )
p6	1009.58(2)	6.07(5)	976.40(5)	5.39(9)	358.23(2)	7.97(8)
p5	1009.53(1)	6.50(1)	975.86(3)	5.54(5)	357.18(1)	7.75(2)
p4	1009.01(1)	6.49(2)	975.61(4)	5.87(7)	357.31(1)	8.26(3)
p3	1008.94(1)	7.34(2)	975.39(4)	6.40(7)	357.09(1)	8.86(4)
p2	1008.85(1)	7.47(3)	975.33(5)	6.32(10)	356.60(9)	8.51(3)
p1	1009.18(1)	7.25(2)	975.65(4)	6.07(7)	357.06(1)	8.14(4)

Note: the errors in bracket are referred to the fit

\*Value measured before polishing

† Value measured just after polishing

§ Value measured two days after polishing end

TABLE S.3. POLISHING EFFECT ON ZIRCON SAMPLE S3

p. analysis	Shift (cm-1)	Normalized shift	Uncertainty norm. shift	Shift (cm-1)	Normalized shift	Uncertainty norm. shift	Distance ( $\mu\text{m}$ )	Normalized Distance	Uncertainty norm. distance
p0	1011.28	0.00	0.18	977.56	0.00	0.18	100	5.00	0.52
p7	1011.34	0.02	0.18	977.63	0.02	0.18	85	4.25	0.44
p13	1011.11	-0.06	0.17	977.31	-0.09	0.17	55	2.75	0.30
p16_bis	1010.53	-0.27	0.16	976.65	-0.34	0.16	45	2.25	0.26
p19	1009.68	-0.58	0.16	976.01	-0.57	0.16	30	1.50	0.20
p36	1010.06	-0.44	0.16	976.36	-0.44	0.16	20	1.00	0.16
p53	1009.04	-0.81	0.17	975.29	-0.84	0.17	15	0.75	0.15
<b>reference</b>	<i>1008.53</i>	<i>-1.00</i>	<i>0.18</i>	<i>974.85</i>	<i>-1.00</i>	<i>0.18</i>			

TABLE S.4: POLISHING EFFECT ON ZIRCON SAMPLE S2

p. analysis	Shift (cm-1)	Normalized shift	Uncertainty norm. shift	Shift (cm-1)	Normalized shift	Uncertainty norm. shift	Distance ( $\mu\text{m}$ )	Normalized distance	Uncertainty nom. distance
2	1013.16	0.00	0.11	979.80	0.00	0.10	90	4.50	0.47
6	1013.13	-0.01	0.11	979.84	0.01	0.10	70	3.50	0.37
8	1012.91	-0.05	0.10	979.40	-0.08	0.10	60	3.00	0.33
9	1012.60	-0.12	0.10	978.92	-0.18	0.09	40	2.00	0.24
27	1010.57	-0.56	0.09	976.98	-0.57	0.09	20	1.00	0.16
reference	1008.53	-1.00	0.18	974.85	-1.00	0.18			

TABLE S.5: POLISHING EFFECT ON COESITE SAMPLE S24

p. analysis	Shift (cm <sup>-1</sup> )	Norm. shift	uncertain y norm. shift	Shift (cm <sup>-1</sup> )	Norm. shift	uncertain y norm. shift	Shift (cm <sup>-1</sup> )	Norm. shift	uncertainty norm. shift	Distance ( $\mu$ m)	Norm. Distance	uncertainty norm. distance
p0	127.21	0.00	0.07	183.84	0.00	0.091	524.18	0.00	0.22	145	14.5	2.9
p1	127.01	-0.03	0.07	183.41	-0.08	0.088	524.03	-0.07	0.22	140	14	2.8
p2	127.20	0.00	0.07	184.09	0.04	0.094	524.30	0.06	0.23	135	13.5	2.7
p3	127.24	0.00	0.07	183.88	0.01	0.092	524.37	0.09	0.23	130	13	2.6
p4	127.41	0.03	0.07	184.10	0.05	0.094	524.43	0.11	0.24	110	11	2.2
p5	127.13	-0.01	0.07	183.71	-0.02	0.090	524.20	0.01	0.22	90	9	1.8
p6	127.44	0.03	0.07	184.25	0.07	0.095	524.64	0.21	0.25	70	7	1.4
p7	127.72	0.07	0.07	184.15	0.06	0.094	524.75	0.26	0.26	50	5	1
p8	124.07	-0.42	0.06	181.35	-0.46	0.079	523.23	-0.43	0.19	30	3	0.6
p9	123.82	-0.46	0.06	181.00	-0.52	0.079	523.37	-0.36	0.20	10	1	0.2
p10	123.06	-0.56	0.06	180.50	-0.62	0.080	522.74	-0.65	0.20	5	0.5	0.1
p11	122.95	-0.57	0.06	180.63	-0.59	0.080	522.82	-0.61	0.19	0	0	0
reference	119.75	-1.00		178.42	-1.00		521.95	-1.00				

TABLE S.6. POLISHING EFFECT VS HYDROSTATIC PRESSURE CALIBRATION

P. analysis	Schift (cm-1)	Delta shift (cm-1)	dw/dP (cm-1/GPa)	Pressure (GPa)	Schift (cm-1)	Delta shift (cm-1)	dw/dP (cm-1/GPa)	Pressure (GPa)	Schift (cm-1)	Delta shift (cm-1)	dw/dP (cm-1/GPa)	Pressure (GPa)
p0	127.21	7.46	7.40	1.01	183.84	5.42	5.26	1.03	524.18	2.23	2.90	0.77
p0	127.01	7.26	7.40	0.98	183.41	4.99	5.26	0.95	524.03	2.08	2.90	0.72
p1	127.20	7.45	7.40	1.01	184.09	5.67	5.26	1.08	524.30	2.35	2.90	0.81
p2	127.24	7.49	7.40	1.01	183.88	5.46	5.26	1.04	524.37	2.42	2.90	0.83
p3	127.41	7.66	7.40	1.04	184.10	5.68	5.26	1.08	524.43	2.48	2.90	0.86
p4	127.13	7.38	7.40	1.00	183.71	5.29	5.26	1.01	524.20	2.25	2.90	0.77
p5	127.44	7.69	7.40	1.04	184.25	5.83	5.26	1.11	524.64	2.69	2.90	0.93
p6	127.72	7.97	7.40	1.08	184.15	5.73	5.26	1.09	524.75	2.80	2.90	0.96
p7	124.07	4.32	7.40	0.58	181.35	2.93	5.26	0.56	523.23	1.28	2.90	0.44
p8	123.82	4.07	7.40	0.55	181.00	2.58	5.26	0.49	523.37	1.42	2.90	0.49
p9	123.06	3.31	7.40	0.45	180.50	2.08	5.26	0.39	522.74	0.79	2.90	0.27
p11	122.95	3.20	7.40	0.43	180.63	2.21	5.26	0.42	522.82	0.87	2.90	0.30
reference	119.75				178.42				521.95			

TABLE S.7. ELASTIC PARAMETERS AT ROOM CONDITIONS FOR ZIRCON AND PYROPE USED FOR FINITE ELEMENT CALCULATIONS

Zircon (anisotropic elastic properties)	C11	C33	C44	C66	C12	C13
	(GPa)					
	423.7	490	113.6	48.5	70.3	149.5
Pyrope (isotropic elastic properties)	K <sub>0T</sub> (GPa)			G <sub>0T</sub> (GPa)		
	163.7			94.0		

TABLE S.8: RESIDUAL PRESSURES FOR THE ZIRCON S2

N. Distance	$\Delta\omega$ 975 (cm <sup>-1</sup> )	$\Delta\omega$ 1008 (cm <sup>-1</sup> )	e <sub>1</sub> -e <sub>2</sub>	e <sub>3</sub>	P <sub>inc</sub> (GPa)
4.5	4.96000	4.63000	-1.162525	-0.44395	0.923
3.5	5.00000	4.60000	-1.1895	-0.40035	0.92645
3.0	4.56000	4.38000	-1.027	-0.4618	0.8386
2.0	4.08000	4.07000	-0.8892	-0.5382	0.7722
1.0	2.13000	2.04000	-0.4888	-0.21595	0.39785

TABLE S.9: RESIDUAL PRESSURE FOR THE ZIRCON S3

N. Distance	$\Delta\omega$ 975 (cm <sup>-1</sup> )	$\Delta\omega$ 1008 (cm <sup>-1</sup> )	e <sub>1</sub> -e <sub>2</sub>	e <sub>3</sub>	P <sub>inc</sub> (GPa)
5.0	2.78000	2.94017	-0.56355	-0.46095	0.52935
4.2	2.78000	2.81077	-0.5928	-0.3588	0.5148
2.7	2.46000	2.58099	-0.4992	-0.38205	0.46015
2.2	1.81000	2.00278	-0.3562	-0.3754	0.3626
1.5	1.16000	1.14690	-0.2717	-0.16445	0.23595
1.0	1.52000	1.52951	-0.3211	-0.19435	0.27885
0.7	0.44000	0.51245	-0.06435	-0.0789	0.0692