

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

4 N. Campomenosi¹, M.L. Mazzucchelli², B.D. Mihailova³, M. Scambelluri¹, R.J. Angel², F.
5 Nestola⁴, A. Reali⁵, M. Alvaro²

6 ¹*Department of Earth Science, Environment & Life, University of Genoa, Corso Europa 26, 16132*
7 *Genoa, Italy.*

8 ²*Department of Earth and Environmental Sciences, University of Pavia, Via A. Ferrata, 1 I-27100*
9 *Pavia, Italy,*

10 ³*Department of Earth Sciences, University of Hamburg, Grindelallee 48, D-20146 Hamburg,*
11 *Germany.*

12 ⁴*Department of Geosciences, University of Padova, Via G. Gradenigo 6, I-35131 Padova, Italy.*

13 ⁵*Department of Civil Engineering and Architecture, University of Pavia, Via A. Ferrata 3, I-27100*
14 *Pavia, Italy*

17 *Corresponding author: matteo.alvaro@unipv.it*

18 **Abstract**

19 Raman spectroscopy provides information on the residual strain state of host-inclusion systems that,
20 coupled with the elastic geobarometry theory, can be used to retrieve the *P-T* conditions of inclusion
21 entrapment. In-situ Raman measurements of zircon and coesite inclusions in garnet from the
22 Ultrahigh-pressure Dora Maira Massif show that rounded inclusions exhibit constant Raman shifts
23 throughout their entire volume. In contrast, we demonstrate that Raman shifts can vary from the
24 center to the edges and corners of faceted inclusions. Step-by-step polishing of the garnet host show
25 that the strain in both rounded and prismatic inclusions is gradually released as the inclusion
26 approaches the free surface of the host. More importantly our experimental results coupled with
27 selected numerical simulations demonstrate that the magnitude and the rate of the strain release
28 depends also on the contrast in elastic properties between the host and the inclusion and on the
29 inclusion crystallographic orientation with respect to the external surface. These results allowed us to
30 give new methodological guidelines for determining the residual strain in host inclusion systems.

31
32 **Keywords:** elastic barometry; inclusion; Raman spectroscopy; zircon; garnet; coesite; Dora Maira
33 Massif; Ultra High Pressure metamorphism;

34 **Introduction**

35 Elastic geobarometry for host-inclusion systems is based on measurements of the
36 residual strains produced during exhumation as a consequence of the contrast in elastic

REVISED VERSION 1

37 properties between the host and the inclusion. The residual strain in the inclusions can be
38 measured by micro-Raman spectroscopy or X-ray diffraction and can be used to provide
39 estimates of pressure and temperature (P - T) conditions for metamorphic rocks that are not
40 dependent on chemical equilibrium (e.g., Rosenfeld and Chase, 1961; Enami et al., 2007;
41 Angel et al., 2015; Anzolini et al., 2018; Murri et al., 2018). Models for elastic geobarometry
42 only apply to the simple case of elastically isotropic host-inclusion pairs with a simple ideal
43 geometry where a small spherical inclusion is trapped in an infinite host (Angel et al., 2015).
44 Recent numerical models showed that any deviations from the idealized geometry
45 significantly affects the estimation of “residual pressure” (Mazzucchelli et al., 2018). Indeed,
46 gradients in non-spherical inclusions have been already reported (e.g. Zhukov and Korsakov,
47 2015; Murri et al., 2018). Moreover, several studies pointed out the effects on the residual
48 “pressure” determination of the inclusion size and its partial exposure with respect to the
49 mineral host surface (e.g. Rosenfeld and Chase, 1961; Enami et al., 2007; Zhang, 1998;
50 Mazzucchelli et al. 2018). Nevertheless, open questions still remain, including: what is the
51 effect of the inclusion anisotropy on the residual strain release? How much can the contrast
52 in properties between the host and the inclusion and their geometry influence the residual
53 strain? Therefore, we propose an alternative way to test the effect of the geometry of the
54 host-inclusion system on the Raman signal and on the calculated residual pressure upon
55 polishing: to collect spectra from selected inclusions with different shape, size and
56 crystallographic orientation, while performing several steps of polishing of the rock thick
57 section to bring the inclusion closer to the external surface of the host.

58 In this manuscript we report the Raman spectra of rounded and elongated zircon
59 inclusions and a rounded coesite inclusion in pyrope from the ultrahigh-pressure (UHP)
60 Alpine Dora Maira Massif measured before and after several subsequent steps of polishing.
61 The measured “residual pressures” are compared with the results of a set of Finite Element

REVISED VERSION 1

62 models following the approach of Mazzucchelli et al. (2018). This allows us to provide new
63 methodological guidelines and examples of correction curves to adjust measurements carried
64 out on faceted and anisotropic inclusions and/or close to the host surface.

65

66

Sample description

67 We analyzed zircon and coesite inclusions within pyrope megablasts and
68 porphyroblasts respectively, from the whiteschist of the Brossasco-Isasca UHP unit in the
69 Gilba locality, whose petrography and petrology were reported by several authors (e.g.
70 Chopin, 1984; Hermann, 2003). Whiteschists occur as lenses inside ortho-gneiss and para-
71 gneiss of the Monometamorphic Complex (data repository) and mainly consist of quartz,
72 phengite, kyanite and porphyroblastic to megablastic pyrope-rich garnet. The Dora Maira
73 whiteschist shows a phengite, garnet and kyanite-bearing foliation that wraps around the
74 garnet megablasts (up to 15 cm across). The latter contain numerous inclusions (from few
75 microns to 1 mm in size) mainly of kyanite, rutile and zircon. Garnet porphyroblasts (up to 2
76 mm in size) within the foliated rock matrix contain rutile, zircon and coesite inclusions.
77 Coesite grains are frequently surrounded by quartz rims and palisade quartz structures
78 (Chopin, 1984), but we only measured the rare monocrystalline unaltered coesite inclusions.
79 For the application of elastic geobarometry we selected garnet-core and rim domains
80 unaltered and free of fractures. In these domains, the coesite and zircon inclusions are
81 surrounded by birefringent haloes (Figure 1), indicating that the structure of the garnet host
82 around the inclusions is anisotropically strained.

83

84

Methods

85 As pointed out previously (Zhang, 1998; Mazzucchelli et al., 2018), only small
86 isolated inclusions far from any free surface of the garnet thick sections (e.g. distance > 3

REVISED VERSION 1

87 radii of the inclusion) do not suffer potential strain release. Therefore, for this study we
88 prepared polished sections of 250-260 μm thickness. We performed Raman spectroscopic
89 measurements only on inclusions at the center of the section with a mean linear size smaller
90 than 50 μm , (i.e. considerably less than the distance to the host surface).

91 Micro-Raman scattering measurements were conducted in backscattering geometry
92 with a Horiba Jobin-Yvon T64000 triple-monochromator spectrometer with a spectral
93 resolution of $\sim 2\text{ cm}^{-1}$ and instrumental accuracy in peak positions of $\sim 0.35\text{ cm}^{-1}$. For each
94 inclusion, a series of spot measurements were carried out along the equatorial plane of the
95 inclusion as shown in Figure 2. Details of the measurements and data processing are given in
96 the supplementary materials.

97 We collected Raman spectra before and after polishing of the garnet hosts by known
98 amounts. The inclusion distance from the surface (i.e. the distance between the equatorial
99 plane of the inclusion and the host external surface) was estimated by means of optical focus
100 coupled with the controlled z-position motorized microscope stage. We repeated the
101 procedure until the inclusion was half-exposed. This allowed us to observe the “real time”
102 evolution of the strains inside the inclusions in terms of changes in the Raman frequencies.
103 Here we show examples of single crystals of zircon: one rounded ($\square 20\text{ }\mu\text{m}$ radius) and one
104 prismatic ($\square 80\text{ }\mu\text{m}$ along the long axis), labelled S2 and S3, respectively and one rounded
105 single crystal of coesite ($\square 15\text{ }\mu\text{m}$ radius, sample S24) in the garnet megablasts and
106 porphyroblasts, respectively. No prismatic or idiomorphic coesite inclusions have been
107 found. Since our inclusions are elastically anisotropic, their orientation with respect to the
108 polishing surface is critical for the interpretation of the results by means of numerical
109 simulations. The idiomorphic zircon grain S3 has the *c* axis inclined with respect to the
110 polishing surface by approximately 20° (estimated optically). Analysis of the peak intensities
111 in the polarized Raman spectra suggests that the rounded zircon grain S2 has its *c* axis

REVISED VERSION 1

112 almost perpendicular to the surface. The coesite crystal S24 was rounded and the absence of
113 pronounced changes in the Raman intensities measured in different scattering geometries
114 makes it impossible to determine its orientation and therefore it was not possible to perform
115 numerical simulations for this inclusion.

116 Finite element simulations have been carried out to support the interpretation of our
117 measurements of zircon inclusions S2 and S3 and to evaluate the effect of the proximity of
118 the inclusion to the external surface of the thick section on the residual strain of the inclusion
119 (procedures as in Mazzucchelli et al., 2018, further details are reported in data repository).
120 Elastic anisotropy has been incorporated in the model for the zircon inclusions. The pyrope
121 host was treated as isotropic because its universal elastic anisotropy index (Ranganathan and
122 Ostoja-Starzewski, 2008) is negligible (i.e. 9×10^{-4}), based on the elastic moduli reported by
123 Sinogeikin and Bass (2002). The use of isotropic elastic properties for the host allows us to
124 neglect the mutual crystallographic orientation of the host and the inclusion. For our
125 purposes, the only relevant orientation is that of the inclusion with respect to the surface of
126 the petrographic section.

127

128

Results and discussion

129 Both rounded and idiomorphic inclusions close to the center of the section display Raman
130 peak positions shifted toward higher wavelengths compared to free reference crystals. Within
131 the instrumental precision ($\pm 0.35 \text{ cm}^{-1}$), the rounded zircon inclusion S2 and the rounded
132 coesite inclusion S24 showed no spatial variation of the Raman peak positions within the
133 inclusions. On the other hand, for idiomorphic crystals (zircon inclusion S3 with well-
134 developed corners and edges) there is a steady increase in the peak positions of about 1 cm^{-1}
135 from the center towards the edges of the inclusions (Figure 2 B). This is a direct
136 consequence of strain heterogeneity in the inclusion, which can be caused by chemical

REVISED VERSION 1

137 zonation, zoned radiation-induced damage and/or an imposed strain gradient. The
138 substitution of elements such as Th, U, or Hf for Zr, may cause expansion (U, Th) or
139 contraction (Hf) of the zircon unit cell (Nasdala et al., 1998), leading to a change in the
140 phonon wavenumbers. However, compositional analysis of the exposed grain performed
141 after the final step of polishing did not reveal any chemical zonation (see supplementary
142 material). Radioactive decay of elements such as U and Th can induce structural damage,
143 leading to Raman peak broadening and a shift towards lower wavenumbers (Binvignat et al.,
144 2018). However, the full-width-at-half-maximum (FWHM) of a given phonon mode for
145 totally entrapped S3 remains the same throughout the entire grain and within the
146 instrumental spectral resolution and is equal to that of well crystalline zircon (Binvignat et
147 al., 2018), thus indicating a high degree of crystallinity throughout the entire grain bulk.
148 Since the zircon inclusion S3 is chemically homogeneous (see Appendix A.1) and well-
149 crystalline, the variable Raman shift in it is due to its faceted shape (Eshelby, 1957), because
150 the edges and corners act as stress concentrators (Zhang, 1998; Mazzucchelli et al., 2018).
151 After polishing the Raman spectra of S3 became homogeneous within the fully exposed part
152 of the sample (Figure 2 B), confirming that the variation in the peak position in a single
153 crystal for all bands was caused by the shape of the crystal.

154 A decrease in the Raman band wavenumbers was measured at the center of the inclusions
155 upon polishing for all the investigated samples of zircon and coesite. As an example, Figure
156 3A shows the B_{1g} mode near 1008 cm^{-1} measured on zircon sample S3 at three different steps
157 of polishing. Strictly speaking, the phonon wavenumbers are directly related to the strain,
158 rather than to the applied pressure. Moreover, for elastically anisotropic materials the same
159 relative volume change can be obtained by different strains, for example as induced by
160 hydrostatic or deviatoric stress. Therefore, the commonly used direct proportionality
161 between the Raman peak positions and residual pressure is a strongly oversimplified

162 assumption (Murri et al., 2018). Nonetheless, if we assume that the change in Raman
163 wavenumber ω is linear with mean stress P (i.e. $\frac{\partial \omega}{\partial P}$ is constant), we can introduce the
164 normalized change in the peak position $\Delta\omega_{norm}$ as a parameter to express the relative
165 release in “pressure” as the inclusion becomes closer to the external surface of the host
166 during polishing:

167

$$\Delta\omega_{norm} = \frac{\left((\omega_{I,d} - \omega_{I,0}) \frac{\partial P}{\partial \omega} - (\omega_{I,\infty} - \omega_{I,0}) \frac{\partial P}{\partial \omega} \right)}{(\omega_{I,\infty} - \omega_{I,0}) \frac{\partial P}{\partial \omega}} = \frac{P_{I,d} - P_{I,\infty}}{P_{I,\infty}} \quad (1)$$
$$= \frac{(\omega_{I,d} - \omega_{I,\infty})}{(\omega_{I,\infty} - \omega_{I,0})} = \Gamma$$

168

169 Where $\omega_{I,0}$ is the wavenumber for a free crystal measured at ambient conditions, $\omega_{I,\infty}$ and
170 $P_{I,\infty}$ are the wavenumber and the corresponding pressure for an inclusion in an infinitely
171 large host (i.e. before the polishing, when the inclusion was far from the surface of the host),
172 while $\omega_{I,d}$ and $P_{I,d}$ are the wavenumber measured on the inclusion and its pressure after
173 each polishing step and associated to a specific normalized distance d (i.e. the distance from
174 the inclusion center to the host external surface divided by the corresponding inclusion
175 radius). Under these assumptions, equation (1) shows that $\Delta\omega_{norm}$ becomes equivalent to
176 the geometrical factor Γ defined by Mazzucchelli et al. (2018).

177 As can be seen in Figure 3 B and C, the normalized change in the peak position $\Delta\omega_{norm}$
178 decreases progressively towards -1 (i.e. the Raman shift becomes equal to that of the free
179 inclusion), when the inclusion approaches the host surface. The trends of “pressure” release
180 estimated from the Raman spectra measured on our zircon samples show the same pattern
181 with those calculated from numerical simulations performed on similar geometries and

REVISED VERSION 1

182 crystallographic orientations (e.g. see the dotted lines in fig. 3 B). However, the experimental
183 data suggest a greater amount of stress release compared to the numerical simulations. For
184 example, at a normalized distance of 1 (inclusion just in contact with the external surface),
185 the calculated stress release is approximately 50%, whereas that obtained from experimental
186 data is about 70% (fig. 3 A). There are at least two contributions to this discrepancy: (i) for
187 non-cubic inclusions, direct conversion of Raman shifts into pressures using a hydrostatic
188 calibration is incorrect; (ii) when the inclusion is close to the surface, strain gradients may be
189 relaxed through plasticity or micro-fractures that are not considered in our purely elastic
190 numerical models. Interestingly, our experiments show that even after partial exposure of the
191 inclusion (i.e. for normalized distances ≤ 1) the Raman shift does not record full strain
192 release (i.e. the inclusion is not at ambient conditions). In Figure 3 C, for example, the
193 polished coesite inclusion still shows 40% of its original residual strain. Finally, the
194 difference in the strain release between zircon and coesite inclusions is probably due to the
195 different contrast in properties with respect the host garnet. Indeed, since coesite is softer
196 than zircon, the host garnet can still retain a greater amount of its residual strain even if half
197 of the inclusion is exposed. This implies the possibility to have thinner hosts for softer
198 inclusions such as coesite or quartz in garnet but, however, the possibility of fracturing
199 during polishing is high (Enami et al., 2007).

200

201

Implications

202 Our measurements show that Raman shift is homogeneous only in rounded inclusions while
203 it is non-homogeneous in faceted ones (Figure 2 A and B), in a full agreement with
204 numerical calculations (Mazzucchelli et al. 2018) and theory (Eshelby, 1957). Therefore,
205 multiple Raman spectra collected on faceted inclusions should not be averaged if their
206 differences are larger than the instrumental peak precision. Instead, to avoid the effects of

REVISED VERSION 1

207 grain shape on Raman peak positions, only Raman spectra measured at the center of the
208 inclusions should be used because there we can apply the geometrical correction (see
209 Mazzucchelli et al., 2018).

210 Our polishing experiments confirm that the Raman shift on the inclusion decreases as the
211 inclusion gets closer to the external surface (Rosenfeld and Chase, 1961; Zhang, 1998;
212 Mazzucchelli et al., 2018). Therefore, only inclusions whose centers are distant more than 4
213 radii (Figure 3 B) from the section surface and internal surfaces of the host should be used. If
214 the Raman peak positions vary from one inclusion to another, even when the inclusions are
215 properly selected, this indicates that some other factor is responsible, such as chemical
216 variation in the host or inclusions, or growth of the host and thus inclusion entrapment under
217 different conditions, such as along a prograde subduction path. More importantly, our
218 results, coupled with our FE numerical simulations, show how anisotropy (i.e.
219 crystallographic orientation of the inclusion with respect to the external surface) and the
220 contrast between the inclusion and host physical properties influences the strain release
221 during polishing. Furthermore, even when an inclusion is exposed at the surface of the host
222 grain, it can still exhibit a variation in the peak position with respect to a free crystal, and
223 thus residual strains and stresses (Figure 3 C). Therefore, partially entrapped grains as a
224 strain free standard should be avoided or chosen very carefully against which to measure the
225 Raman shifts of unexposed inclusions.

226 Finally, as an example, if we calculate from our experimental Raman shift values the strain
227 and then the mean stress in the inclusion after subsequent polishing steps, following the
228 approach given by Murri et al. (2018), the zircon S3 has an initial residual pressure (P_{inc})
229 before polishing of 0.5 GPa. After 55 microns of polishing (1.5 of normalized distance in
230 figure 3 B), when the inclusion is still buried in its garnet host, the P_{inc} drops to 0.2 GPa. A
231 value of 0.06 GPa is recorded when the inclusion is half exposed. For zircon S2 the initial

REVISED VERSION 1

232 P_{inc} was about 0.9 GPa and about 0.3 GPa when the inclusion was just touching the external
233 surface of the host. In the supplementary material a table showing the evolution of the P_{inc} as
234 function of the polishing for the two zircon inclusions is reported (Table S.8). For coesite no
235 reliable data are available to give the strain state of the inclusion from the Raman peak
236 positions.

237

238

Acknowledgments

239

240 This project received funding from the European Research Council (ERC) under the
241 European Union's Horizon 2020 research and innovation program grant agreements 714936
242 to Alvaro and ERC Starting Grant n. 307322 to Nestola. Alvaro has also been supported by
243 the MIUR-SIR (Ministry of Education, University and Research–Scientific Independence of
244 Young Researchers, Italy) grant MILE DEEP (Mineral Inclusion Elasticity for a New Deep
245 Subduction Geobarometer; RBSI140351). Campomenosi acknowledges the University of
246 Genova for funding. The authors are grateful to Peter Stutz, Hamburg, for thin-section
247 polishing and to Alessandra Gavoglio and Paolo Campanella, Genova, for the thin-section
248 preparation, Stefanie Heidrich, Hamburg, and Laura Negretti, Genova, for help with electron
249 microprobe analysis. We thank Ian Swainson for the precious editorial work and the three
250 reviewers for their fruitful suggestions and comments.

251

252

References

253 Angel, R.J., Nimis, P., Mazzucchelli, M.L., Alvaro, M., and Nestola, F., 2015, How large are
254 departures from lithostatic pressure? Constraints from host-inclusion elasticity.
255 *Journal of Metamorphic Geology*, 33, 801–813.

256 Anzolini, C., Prencipe, M., Alvaro, M., Romano, C., Vona, A., Lorenzon, S., Smith, E. M.,
257 Brenker, F. E., Nestola, F., 2018, Depth of formation of super-deep diamonds:

REVISED VERSION 1

- 258 Raman barometry of CaSiO₃-walstromite inclusions. American Mineralogist, 103(1):
259 69-74.
- 260 Chopin, C., 1984, Coesite and pure pyrope in high-grade blueschists of the Western Alps: a
261 first record and some consequences. Contributions to Mineralogy and Petrology, 86,
262 107–118.
- 263 Binvignat F. A. P., Malcherek T., Angel R. J., Paulmann C., Schlüter J. Mihailova B. D.,
264 2018
265 Radiation-damaged zircon under high pressures. Physics and Chemistry of
266 Minerals.
- 267 Enami, M., Nishiyama, T., and Mouri, T., 2007, Laser Raman microspectrometry of
268 metamorphic quartz: A simple method for comparison of metamorphic pressures.
269 American Mineralogist, 92, 1303–1315.
- 270 Eshelby, J. D., 1957, The determination of the elastic field of an ellipsoidal inclusion and
271 related problems. Proceedings of the Physical Society of London, Series A, 241, 376-
272 396.
- 273 Hermann, J., 2003, Experimental evidence for diamond-facies metamorphism in the Dora-
274 Maira massif. Lithos, 70, 163-182.
- 275 Mazzucchelli, M.L., Burnley, P., Angel, R.J., Morganti, S., Domeneghetti, M.C., Nestola, F.,
276 and Alvaro, M., 2018, Elastic geothermobarometry: Corrections for the geometry of
277 the host-inclusion system. Geology, 46(3), 231-234.
- 278 Murri M., Mazzucchelli M. L., Campomenosi, N., Korsakov, A. V., Prencipe, M.,
279 Mihailova, B. D., Scambelluri, M., Angel, R. J., and Alvaro, M., 2018 Raman elastic
280 geobarometry for anisotropic mineral inclusions. American Mineralogist, in press

REVISED VERSION 1

- 281 Nasdala, L., Pidgeon, R.T., Wolf, D., and Irmer, G., 1998, Metamictization and U-Pb
282 isotopic discordance in single zircons: a combined Raman microprobe and SHRIMP
283 ion probe study. *Mineralogy and Petrology*, 62, 1–27.
- 284 Rosenfeld, J.L. & Chase, A.B., 1961. Pressure and temperature of crystallization from elastic
285 effects around solid inclusion minerals? *American Journal of Science*, 259, 519-541.
- 286 Sinogeikin, S. V., and Bass, J.D., 2002, Elasticity of pyrope and majorite-pyrope solid
287 solutions to high temperatures. *Earth and Planetary Science Letters*, 203, 549-555.
- 288 Zhang, Y., 1998. Mechanical and phase equilibria in inclusion–host systems. *Earth and*
289 *Planetary Science Letters*, 157, 209-222.
- 290 Zhukov, V. P., & Korsakov, A. V. (2015). Evolution of host–inclusion systems: a visco–
291 elastic model. *Journal of Metamorphic Geology*, 33(8), 815-828.

292

293 **Figure captions**

294 **Figure 1.** A polished pyrope megablast section with partial talc + chlorite alteration along
295 fractures and rims. The red square shows an example of a mm-sized fracture-free garnet area
296 selected for this study, in which zircon and coesite crystalline inclusions exhibiting strain-
297 induced birefringent haloes in the surrounding host have been found.

298

299 **Figure 2.** Position of the Raman peak $A_{1g} \sim 975 \text{ cm}^{-1}$ in a rounded (A) and an idiomorphic
300 (B) zircon crystal before and after the final step of polishing. The solid lines in the plots are
301 guides for the eye; the dashed line in (B) traces the data points measured after two days of
302 final exposure of the grain.

303

304 **Figure 3.** (A) Raman scattering arising from the antisymmetric SiO_4 stretching (the B_{1g}
305 crystal phonon mode $\sim 1008 \text{ cm}^{-1}$) measured when the grain S3 was fully entrapped (red

REVISED VERSION 1

306 line), at an intermediate stage of polishing (yellow), and when the inclusion was exposed at
307 the final stage of polishing (green line). The numbers are the measured Raman shifts. (B)
308 Measured normalized wavenumber shifts $\Delta\omega_{\text{norm}}$ for zircon S2 (green circles) and zircon S3
309 (blue squares) versus the normalized distance d to the host surface along with gaussian fits to
310 the corresponding data $A_{1g} \sim 975$ and $B_{1g} \sim 1008 \text{ cm}^{-1}$ data sets (solid lines) as well as the
311 calculated geometrical factor Γ (dashed lines) from the FE model; $\Delta\omega_{\text{norm}}(d)$ and $\Gamma(d)$ show
312 the same trend within uncertainties. (C) Measured $\Delta\omega_{\text{norm}}(d)$ (red circles) and a gaussian fit
313 to $A_{1g} \sim 119$ and $\sim 521 \text{ cm}^{-1}$ (solid line) for S24 coesite inclusion
314
315





