

Reaction-induced volume change triggers brittle failure at eclogite facies conditions

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Philippe Yamato, Thibault Duretz, M. Baïsset, Cindy Luisier. Reaction-induced volume change triggers brittle failure at eclogite facies conditions. Earth and Planetary Science Letters, 2022, 584, pp.117520. 10.1016/j.epsl.2022.117520. insu-03638866

HAL Id: insu-03638866 https://insu.hal.science/insu-03638866

Submitted on 13 Apr 2022

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2	conditions		
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12	Highlights:		
13	- Densification due to eclogitization reaction can generate significant shear stresses		
14	- Degree of reaction overstepping impacts the amount of generated shear stresses		
15	- Reaction-induced stresses can trigger brittle failure at high-pressure conditions		
16	- Negative volume change and associated brittle failure enhance reaction propagation		
17			
18	Keywords:		
19	volume change, High-Pressure metamorphism, frictional plasticity, numerical modelling		
20			
21			

22 Abstract

23

24 Metamorphic reactions can lead to important changes in rock strength and density. Eclogitization 25 constitutes one of the most emblematic transformations in continental subduction zones, where 26 conversion of lower crustal rocks into eclogite facies rocks correlates with the occurrence of 27 seismogenic events. The relationship between eclogitization and seismicity has been highlighted in 28 several studies, but the processes that trigger brittle failure remain highly debated. Indeed, whether the change in density (from ~2850 kg.m⁻³ to ~3300 kg.m⁻³) or the change in rheology can lead to 29 30 embrittlement is still enigmatic. Here we show that eclogitization-induced volume change occurring 31 out of equilibrium can, by itself, generate sufficient shear stress to fail the rocks at high-pressure 32 conditions. Intermediate-depth earthquakes in continental subduction zones could therefore be 33 explained by volume changes, even without considering rheological modifications induced by 34 mineral reactions. Our results also indicate that interplay between negative volume change and frictional plastic yielding can enhance the propagation of the eclogitization process by a runaway 35 36 mechanism as long as the reaction is not limited by the lack of reactants.

37

38 **1. Introduction**

39

40 When buried at depth in convergent zones, rocks are subjected to pressure (P) and temperature (T)41 changes. Depending on their chemical composition and fluid content, the mineral assemblages and 42 proportions evolve toward more thermodynamically stable assemblages at increasing P-T43 conditions (Spear, 1993). Eclogitization of the oceanic and continental crust involves a large 44 increase in solid density and fluid release, which have significant impacts on tectonic deformation 45 and long-term lithosphere dynamics (e. g., Kirby et al., 1996; Hacker et al., 2003; Jung et al., 2004; Hetenyi et al., 2007; 2021; Malvoisin et al., 2020). In addition, there is growing evidence 46 47 supporting a genetic link between eclogitization reactions and short-term geological processes, such

as the generation of seismic events at intermediate depth (Fig. 1a, b, Hacker et al., 2003; Jung et al.,
2004; Austrheim and Boundy, 1994; Hetenyi et al., 2007; Nakajima et al., 2013; Shi et al., 2018;
Incel et al., 2019).

51 However, it is still unclear and there is no consensus yet on the mechanism responsible for this 52 behaviour. Indeed, even the strongest mineral phases are expected to deform in a ductile rather than brittle manner above 700°C and 1 GPa of confining pressure, and for a strain rate of 10⁻¹⁴ s⁻¹ (e.g. 53 dry plagioclase flow laws, Rybacki and Dresen, 2000; 2004). We thus face a chicken-and-egg 54 55 problem: it is hard to decipher whether brittle deformation is induced by metamorphic reactions or 56 if the reaction itself triggers embrittlement at high pressure. Several studies have addressed this 57 issue by proposing either of these scenarios. On one hand, reaction-induced embrittlement has been 58 proposed to be caused by (i) the change in strength of the newly formed reaction products (grain-59 size reduction, nucleation and/or growth of weaker phases, Stünitz and Tullis, 2001; John et al., 60 2009; Thielmann et al., 2015; Incel et al., 2017), (ii) dehydration of the transforming rocks leading to hydrofracturing through a pore fluid pressure increase (Hacker et al., 2003; Jung et al., 2004, 61 62 Hetényi et al., 2007; 2021; Alvizuri and Hetényi, 2019), and (iii) volume change (McGarr, 1976; Pennington, 1984; Kirby et al., 1996; Malvoisin et al., 2017; 2020). On the other hand, it has been 63 proposed that brittle fracturing could be triggered by transient high stress conditions over very short 64 65 timescales, leading to external fluid infiltration and subsequent transformation of the granulite into eclogite (e.g., Jamtveit et al., 2018). In the latter case, brittle failure at intermediate depths is 66 induced in response to remote seismic events occurring in the seismogenic zone at shallower levels 67 68 (Jamtveit et al., 2018), while in the other aforementioned scenarios, brittle failure occurs in situ as a 69 consequence of a reaction-induced stress perturbation. Whatever the mechanism responsible for 70 embrittlement, it is also plausible that the deformation of the lower continental crust results from a 71 cyclic interplay between fracturing-induced reaction and reaction-induced fracturing involving 72 successive stages of fluid pumping and release. Another mechanism that has been proposed to explain embrittlement is volume change. Although embrittlement triggered by diminishing solid 73

density reactions (e. g., serpentinization, melting) has already been suggested (e. g., Kelemen and Hirth, 2012; Vrijmoed et al., 2009; Schmalholz et al., 2020; Malvoisin et al., 2021) and studied using numerical models (Malvoisin et al., 2017; Ulven et al., 2014), densification has received less attention. Moreover, due to complex numerical issues, only recently could frictional plasticity be robustly included into models that account for non-linear visco-elasto-plastic deformation of heterogeneous and compressible materials (e. g., Duretz et al., 2021).

80 Lower crustal rocks consist of amphibolite to granulite facies rocks, whose densification is mainly 81 controlled by the transformation of plagioclase into omphacite (Fig. 1c-e). It is associated with an important density change of ~ 400-500 kg.m⁻³ (Fig. 1f) and with a transient variations of material 82 83 strength (Bras et al., 2021). Another major characteristic of densification reactions in fluid under-84 saturated lower crustal rocks, such as amphibolites and granulites, is that they usually take place far 85 from the predicted thermodynamic equilibrium (e.g., Austrheim, 1987; Wayte et al., 1989; Wain et 86 al., 2001; Jackson et al., 2004; Hetényi et al., 2007, 2021). Metastability of such rocks in subduction 87 zones has been discussed in several studies (Lund et al., 2004; Young and Kylander-Clark, 2015; 88 Palin et al., 2017) and fast rock transformation, after a delay corresponding to a reaction overstep of 89 several kbars, has been proposed as a cause of intermediate-depth earthquakes (Dennis and Walker, 90 1965; Jamtveit et al., 2016; Incel et al., 2019; Hetényi et al., 2007; 2021).

91 Here, we investigate the mechanical response to densification of the lower crust using thermo-92 mechanical numerical modelling. The aim of this study is therefore to quantify the amount of shear 93 stress that can be generated by the solid volume change induced by eclogitization, by taking into 94 account reaction pressure overstepping (Fig. 2 a, b). We consider the eclogitization as a 95 densification reaction and voluntary ignore the potential strength variations induced by this 96 transformation (i.e. reaction softening/hardening). Our study can then be considered as an end-97 member case, in which adding a softening mechanism would further amplify strain localisation that 98 is already generated by densification. We show that, in deforming rocks, the stress generated during

99 densification can indeed overcome the yield stress, hence generating frictional plastic yielding in

100 rocks that would otherwise be in the ductile realm.

101

102 **2. Methods**

103 **2.1. Modelling strategy and validation**

We designed numerical models to simulate the progress of eclogitization of a radial inclusion enclosed in a granulitic material (Fig. 2c, d) placed at metastable conditions (i.e., at a background pressure (P_{BG}) larger than the pressure of the reaction (P_r) predicted by equilibrium thermodynamics) for a fixed temperature (Fig. 2a, b). The initial degree of overstepping is set by initially placing the whole model at a background pressure of 500 MPa (for the reference model) above the pressure of reaction (i.e., $P_{BG} = 2.0$ GPa and $P_r = 1.5$ GPa).

110 First, a one-dimensional (1D) model (Fig. 2c) involving linear viscous rheology was used to extract 111 the maximum shear stress obtained during the densification of a segment of the model (r_{inc}) placed in metastable conditions (i.e., $P_{BG} > P_r$), assuming no background strain rate (see section 2.3). A 112 constant linear viscous rheology ($\eta = 10^{22}$ Pa.s) is used throughout the model. Parameters are given 113 114 in Table 1. This model allowed us to perform an intensive parametric study on the following parameters: degrees of overstepping ($\Delta P_{\rm m}$), density variation ($\Delta \rho$), shapes of density evolution (d_{Pr}), 115 116 reaction kinetics (τ_k) , shear modulus (G), bulk modulus (K), and linear viscosities (η). Results of 117 this parametric study are presented in Supplementary Figure 1.

118 Two-dimensional (2D) models (Fig. 2d), built upon the 1D models, were used to incorporate the 119 effect of background strain rate and to account for visco-elasto-viscoplastic (V-E-VP) rheologies 120 (see section 2.4), allowing to better quantify the amount of brittle failure and its spatial evolution.

121 Both 1D and 2D models were tested against an analytical solution based on the approach of Lee and

122 Tromp (1995; see section 2.2. and Supplementary Figure 2). Matlab scripts to solve the analytical

solution and to reproduce the 1D model are provided in the Supplementary Materials. The results of

the 1D and 2D models are identical and both converge with increasing grid resolution (seeSupplementary Figure 3).

126

127 **2.2. Analytical solution**

The analytical solution was developed following the method presented in Lee and Tromp (1995). To allow for a direct comparison with the 2D models, the original solution was modified to account for cylindrical coordinates. Displacement, pressure and stress fields are caused by the instantaneous density change (from ρ_i to ρ_f) of a cylindrical inclusion of radius r_{inc} embedded in an elastic matrix. The associated volume change generates a self-induced stress, which is proportional to the density change through a constant *C* that can be expressed as:

134
$$C = -\frac{1}{2} \ln \frac{\rho_f}{\rho_i} \tag{1}$$

135 The radial displacement vector (u_r) , in cylindrical coordinates, can then be computed analytically 136 for a variable radial distance *r* using the following equation:

137
$$u_r = Ar - B\frac{1}{2r} \tag{2}$$

138 where A and B, that depend on C, are constants. The latter may be determined from the application 139 of boundary and transmission conditions associated with material interfaces (i.e. inclusion for $r \leq$ 140 r_{inc} and matrix for $r > r_{inc}$, see script SphereInHole_cylindrical.ipynb for more details). The 141 inclusion and the matrix are both considered elastic with similar material properties (i.e. bulk 142 modulus K=40 GPa and shear modulus G=30 GPa). However, the proposed analytical solution 143 could also be used for different elastic properties between the reacting inclusion and the matrix. The 144 Matlab script corresponding to this analytical solution is provided in supplementary file 145 (AnalyticalSolution.m). It allows to test the validity of both the 1D and the 2D model used in our 146 study (See Supplementary Figure 2).

147

148 **2.3. Description of the 1D model**

The 1D model used in this study solves the continuity and momentum equations in the [r, p] polar coordinates. In this coordinate system, we consider the volume change affecting a radial inclusion (with a radius r_{inc}) embedded in a radial domain (Fig. 2c). In the absence of body forces and inertia, the continuity and momentum equations are expressed as:

153
$$\frac{d\ln(\rho)}{dt} = -\frac{1}{r}\frac{\partial(rV_r)}{\partial r}$$
(3)

154 and:

155
$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \left(\sigma_{rr} - \sigma_{pp} \right) = 0 \tag{4}$$

156 where ρ is the density, *V* the velocity, *r* the distance from the center of the model, and σ_{rr} and σ_{pp} 157 are the normal stress in *r* and *p* direction, respectively. By definition, total stresses (σ_{rr} and σ_{pp}) 158 can be decomposed as:

159
$$\begin{cases} \sigma_{rr} = -P + \tau_{rr} \\ \sigma_{pp} = -P + \tau_{pp} \end{cases}$$
(5)

160 where *P* is the pressure and τ_{rr} and τ_{pp} , the deviatoric stresses. Note that here stresses are defined 161 as negative in compression. Material constituting the inclusion and the matrix are defined with 162 visco-elastic rheology (see parameters in Table 1) considering a linear viscosity (η) and a shear 163 modulus (*G*). Deviatoric stresses can therefore be computed as:

164
$$\begin{cases} \tau_{rr} = 2\eta_{ve}\dot{\varepsilon}'_{rr} \\ \tau_{pp} = 2\eta_{ve}\dot{\varepsilon}'_{pp}, \end{cases}$$
(6)

165 where $\dot{\varepsilon}'_{rr}$ and $\dot{\varepsilon}'_{pp}$ are the effective deviatoric strain rate components, and η_{ve} corresponds to an 166 effective visco-elastic modulus expressed as follow:

167
$$\eta_{ve} = \left(\frac{1}{\eta} + \frac{1}{G\Delta t}\right)^{-1},\tag{7}$$

168 where Δt corresponds to the time step used in the model for time discretisation. The effective visco-169 elastic deviatoric strain rate components are expressed as:

170
$$\begin{cases} \dot{\varepsilon}'_{rr} = \dot{\varepsilon}_{rr} + \frac{\tau^{0}_{rr}}{2G\Delta t} \\ \dot{\varepsilon}'_{pp} = \dot{\varepsilon}_{pp} + \frac{\tau^{0}_{pp}}{2G\Delta t} \end{cases}$$
(8)

171 τ_{rr}^{0} and τ_{pp}^{0} corresponding to the deviatoric stresses obtained in the previous time step (see Duretz 172 et al., 2021). The driving force in the model is only controlled by the volume change associated 173 with the density change. Motion occurs because the initial pressure (P_{BG}) is higher than the pressure 174 of reaction (Pr). The reaction progress (see Fig. 2b), depends on pressure P and is expressed as a 175 cumulative distribution function (CDF) and takes the following form:

176
$$X_{eq} = 1 - \frac{1}{2} \left(\operatorname{erfc} \left(\frac{P - P_r}{d_{P_r}} \right) \right)$$
(9)

177 where P_r is the "pressure of reaction" (reaction line on Fig. 2a) and d_{Pr} corresponds to a standard 178 deviation of the CDF controlling the density change sharpness (Fig. 2b). At a given *P*, the value of 179 X_{eq} computed using (9) therefore corresponds to a value at equilibrium. In order to introduce a 180 reaction kinetics, the value of *X* considered is computed implicitly using:

$$\frac{dX}{dt} = \frac{X_{eq} - X}{t_k} \tag{10}$$

182 t_k being the kinetic parameter that defines the characteristic reaction time. The reference density is 183 then computed at each time step as:

184
$$\rho_0 = X \rho_{0f} + (1 - X) \rho_{0i} \tag{11}$$

185 where ρ_{0i} and ρ_{0f} corresponds to the initial reference density (2850 kg.m⁻³ for the granulite) and 186 the final reference density (3250 kg.m⁻³ for the eclogite), respectively. Density introduced in 187 continuity equation includes pressure dependency and therefore corresponds to:

188
$$\rho = \rho_0 \exp\left(\beta P\right) \tag{12}$$

where $\beta = 1/K$, is the compressibility (see Table 1). Note that thermal expansivity is not considered and temperature is kept constant throughout the simulations. At each time step, the equations (3-4) are discretized using a staggered finite difference scheme and solved using a pseudo-transient solving strategy (e.g. Duretz et al., 2019). The mesh is advected in a Lagrangian manner following the obtained velocity field. The Matlab script corresponding to this code is provided in supplementary file (Numerics1D_polar.m). It allows to run the 1D reference model and can thus be used to reproduce Figures 3g-i.

197 **2.4. Description of the 2D model**

The 2D thermo-mechanical simulations were carried out using the code MDoodz6.0, which accounts for a V-E-VP rheological model (Duretz et al., 2021). The continuity and momentum equations are solved in 2D Cartesian [x,y] coordinates, neglecting both gravity and inertial terms, such as:

202
$$\frac{d\ln(\rho)}{dt} = -\frac{\partial v_i}{\partial x_i}$$
(13)

203
$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{14}$$

204 The heat transfer equation is expressed as:

205
$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial x_i} \left(k \frac{\partial T}{\partial x_i} \right) + Q_s \tag{15}$$

where k is the conductivity and C_p the heat capacity. Q_s corresponds to viscoplastic dissipation. Note that heat transfer does not affect our results: the temperature remains constant at the considered spatio-temporal scale.

209 The partial differential equations are discretised using a staggered finite difference scheme and 210 markers-in-cell method (Gerya and Yuen, 2003). The non-linear mechanical equations are solved 211 using a full Newton-Raphson method with analytical derivation of the Jacobian (see Duretz et al., 212 2021). Successive Newton corrections are computed using a direct-iterative scheme that relies on 213 Powell-Hestenes iterations, Cholesky factorization of the symmetrised Jacobian operator and 214 Generalized Conjuguate Residual (Räss et al., 2017). The optimal Newton step is computed via a 215 direct line-search globalization procedure (Duretz et al., 2015). Marker positions are evolved forward in time using a fourth order (in space) Runge-Kutta scheme. The Courant number is set to 216 217 0.2. The implementation of the V-E-VP rheological model follows Yamato et al. (2019) and Duretz et al. (2021). The contribution of each deformation mechanism is computed iteratively to satisfy the 218 219 following Maxwell model (e.g., Popov & Sobolev, 2008):

220
$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{v} + \dot{\varepsilon}_{ij}^{e} + \dot{\varepsilon}_{ij}^{vp}$$
(16)

where the v, e and vp superscripts refer to the viscous, elastic, and visco-plastic (frictional) contributions to the total strain rate. In contrast to the 1D model, a dislocation creep flow law is considered in the 2D model. The flow stress (τ_v) is thus stress and thermal dependent and is expressed as:

225
$$\tau_{\rm v} = 2F_{\rm pwl}A^{-\frac{1}{n}}\exp\left(\frac{Q}{nRT}\right)\dot{\varepsilon}_{\rm II}^{\frac{1}{n}}$$
(17)

where *n*, *A*, and *Q* are the dislocation creep parameters of the material (see Table 1) and *R* is the universal gas constant ($R = 8.314510 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$). F_{pwl} corresponds to the correction factor (e.g., Schmalholz & Fletcher, 2011) for invariant formulation relative to the type of experiments used for calibration (here axial compression), such as:

230
$$F_{\text{pwl}} = \frac{1}{6} 2^{\frac{1}{n}} 3^{\frac{n-1}{2n}}.$$
 (18)

In contrast to the 1D simulations, the 2D simulations include the effect of frictional rheology. To this end a viscoplastic Drucker-Prager rheological model is employed³⁵. The yield function is expressed as:

234
$$F = \tau_{\rm II} - P \sin \varphi - C \cos \varphi - 2\eta_{\rm vp} \dot{\varepsilon}_{\rm II}^{\rm vp}$$
(19)

where $\tau_{\rm II}$ is the deviatoric second stress invariant, *P* is the pressure, *C* is the cohesion and φ is the friction angle. The viscoplastic parameter, $\eta_{\rm vp}$, is set such that the overstress $(2\eta_{\rm vp}\dot{\epsilon}_{\rm II}^{\rm vp})$ is on the order of 0.1 MPa (i.e. $\eta_{\rm vp} = 5 \times 10^{18}$ Pa.s for $\dot{\epsilon}_{\rm BG} = 10^{-14}$ s⁻¹) in our simulations. Tests of convergence for 2D models involving plasticity can be found in Supplementary Figure 5. The effect of plastic dilation is neglected and the plastic flow potential (*Q*) thus simply reads as $Q = \tau_{\rm II}$. The reaction progress law and reaction kinetics are included in a similar manner as in the 1D code described above (see eq. 9 to 12).

242

243 **2.5.** Choice of parameters for reference models

244 In this study, eclogitization is restricted to a progressive densification process (Fig. 2b). The choice of parameters for defining a reference model is based on data from granulite to eclogite 245 246 transformation, that has been intensively studied in the Bergen Arcs. Based on recent chemical data and P-T estimates performed in Holsnøy (Bhowany et al., 2018), we set P_r for the granulite to 247 eclogite transformation at 1.5 GPa for a temperature of 680°C. A d_{P_r} value of 700 MPa was chosen 248 249 as it seems to be in good agreement with the density evolution that encompass several reactions occurring with a P increase (Bras et al., 2021, Fig. 1f). Thermodynamic modelling providing the 250 Fig.1f was performed using Perple_X_6.9.1 (Connolly 1990; 2009) and the internally consistent 251 thermodynamic database hp62ver.dat (Holland and Powell, 2011). The solution models are for 252 feldspar (Furhman and Lindsley, 1988), garnet (White et al., 2014), clinopyroxene (Green et al., 253 254 2007), clinoamphibole (Green et al., 2016), epidote (Holland and Powell, 2011), white mica (White et al., 2014), and melt (Green et al., 2016). Bulk composition used corresponds to sample 255 HOL7C_2014 (Bhowany et al., 2018). A difference in density of 400 kg.m⁻³ using a reference 256 density of 2850 kg.m⁻³ for the granulite (X=0) and of 3250 kg.m⁻³ for the eclogite (X=1) appears 257 also in good agreement with previous studies (Austrheim 1987; Hetenyi et al., 2007). The kinetic 258 parameter t_k has been fixed to 100 yrs as there are arguments that granulite to eclogite 259 transformation is rather a fast process (Malvoisin et al., 2020). The choice of the anorthite dry 260 (Rybacki and Dresen, 2000) was stimulated by the fact that initial material corresponds to dry 261 262 granulite. K and G values (Motra and Zertani, 2018). For 2D model involving plasticity, cohesion and friction angle were set to 50 MPa and 30°, as they correspond to an extrapolation of Byerlee's 263 (1978) data at high pressure. The strain rate used in the 2D reference model is 10^{-14} s⁻¹. 264

265

266 **3. Results**

267 **3.1. Results from the reference model**

Figure 3 displays the results obtained in absence of background strain rate and for a linear viscosity set to 10^{22} Pa.s. It shows that reaction-induced volume change affects both shear stress and pressure fields. Shear stresses (τ_{II}) generated by the negative volume change of the inclusion are distributed in a radial configuration around the inclusion (Fig. 3a-c). A fast, transient and important shear stress increase, larger than 500 MPa, occurs in the vicinity of the reacting area at a time close to the onset of reaction (Fig. 3a). After reaching a maximum value (here of ~0.6 GPa), shear stresses then decrease following a Maxwell-type relaxation (Dabrowski et al., 2015) until they become null once equilibrium density is reached.

276 Simultaneously, the densification reaction induces a pressure decrease in both the matrix and the 277 inclusion (Fig. 3 d-f). In the inclusion, there is first a rapid pressure drop (see Fig. 3d compared to 278 the 2.0 GPa initial pressure in both inclusion and matrix, and green line in Fig. 3g-h), followed by a 279 consecutive pressure increase to reach the same pressure as in the matrix (Fig. 3g, h). The pressure 280 decrease in the matrix is smoother (black line in Fig. 3g-h). It is associated to the increase in matrix 281 volume accommodating the shrinking of the inclusion, to satisfy mass conservation. An important 282 point to note is that the reaction stops as soon as both the inclusion and the matrix reached the same density, since our model is only driven by density change, which is not necessarily the one 283 284 predicted for the reaction to be complete (i.e., *X*=1).

285 As the value of the maximum shear stress reached $(max(\tau_{II}))$ constitutes a useful metric that 286 indicates whether reaction-induced volume change can lead to rock failure, we have tracked this 287 value through a complete parametric study (see Supplementary Figure 1). Figure 4a shows the 288 effect of pressure overstepping and density change associated to the metamorphic reaction on the value of $max(\tau_{II})$. The results show that density variations produce shear stress. They also show that 289 290 when a metamorphic reaction is associated with a change in density larger than a few tens of kg.m⁻³, pressure overstepping always leads to shear stress generation, and that the larger the density change 291 292 is, the higher the effect of the overstepping is.

293 The proportion of reacting material is also a key factor (Fig. 4b). Maximum shear stress is reached 294 when the amount of initial reacting material is small (<10%) in comparison to the total amount of

295 material. If the initial reacting area is higher than 20-30%, the maximum shear stress reached is 296 much less important.

297

298 **3.2. Influence of densification on frictional plastic shear banding**

The mechanical consequences of volume changes in an isoviscous host-inclusion system are different from that in host-inclusion systems involving viscosity contrasts and subjected to shear (e.g. Schmid and Podladchikov, 2003; Moulas et al., 2014, Luisier et al., 2019). Figure 5 compares pressure and shear stress fields obtained for models including reaction-induced volume change (Fig. 5a, b) with models involving a viscosity ratio of 1000 between inclusion and matrix (Fig. 5 c, d), under a background strain rate of 10^{-14} s⁻¹.

305 In Figure 5a, inclusion and matrix have the same viscosity and frictional plasticity is not activated. 306 In this case, there is no significant change in pressure around the inclusion. The shear stress (τ_{II}) 307 generated by the negative volume change of the inclusion is radial (see Fig. 3a), but because of the pure shear background strain rate (horizontal shortening and vertical stretching), the shear stress 308 309 field is different in vertical and horizontal direction. τ_{II} values are higher in the vertical direction 310 where shear stresses due to the volume change and shear stresses due to stretching are in the opposite sense. For the same reason, τ_{II} values are smaller in the horizontal direction where 311 312 shortening accompanies the shrinking of the inclusion. When frictional plasticity (i.e. pressure dependent) is accounted for (Fig. 5b), we observe that plastic yield stress in matrix is reached in the 313 area undergoing stretching (where τ_{II} values are high) whereas it is not reached in the area 314 315 undergoing shortening (where τ_{II} values are low). The regions undergoing plastic deformation 316 (contoured in white in Fig. 5b) are located close to the reacting inclusion in the stretching direction. 317 Figure 5c displays pressure and shear stress field obtained for a model using the same parameters as 318 in Fig. 5a, except that (i) there is no volume change and (ii) inclusion and matrix have different viscosities (viscosity 1000 times weaker in the inclusion). In this case, the shear stress field is 319 320 identical in vertical and horizontal directions, but the pressure field is not. Due to the presence of a 321 weak inclusion, a pressure increase occurs in the matrix close to the inclusion in the vertical 322 direction (parallel to stretching). In the horizontal direction, the pressure decreases. Pressure and 323 shear stress fields are therefore drastically different than in the previous case involving volume 324 changes without viscosity contrast. In the "viscosity-contrast" case, shear stress is maximum where 325 the pressure is the lowest in the matrix, close to the inclusion in horizontal direction. These areas 326 constitute favourable locations for frictional plastic yielding. In the vertical direction, because of 327 locally higher pressure values, a larger shear stress is required to reach the yielding. This is the 328 reason why the parts undergoing plastic deformation (white contours in Fig. 5d) are located close to 329 the reacting inclusion in the shortening direction, in the case where plasticity is switched on.

In Figure 5, viscosities are considered stress dependent with a stress exponent n=3. Even if n is known to affect relaxation time and pressure evolution (Dabrowski et al., 2015), performing the same models considering a constant viscosity with n=1 does not drastically change the results concerning matrix deformation over the considered time scale (see Supplementary Figure 4).

334

335 **3.3. Brittle failure in ductile realm**

Our results show that depending on ΔP_m , the amount of shear stress produced $(\max(\tau_{II}))$ by 336 337 considering only reaction-induced volume change is significant (Fig. 4). For a given material, at a fixed pressure-temperature-strain rate (P-T- $\dot{\varepsilon}$) conditions in the ductile field, shear stress (τ_v) 338 339 supported by this material is below the yield stress value (τ_v) required to fail (Fig. 6a). By 340 definition, this difference in stress $\Delta \tau$ (with $\Delta \tau = \tau_v - \tau_v$) can be overcome by (1) increasing strain 341 rate, (2) decreasing pressure and/or (3) decreasing temperature. We here show that shear stresses 342 resulting from reaction-induced volume change can also overcome $\Delta \tau$ and thus trigger yielding. The 343 occurrence of ductile and brittle deformation is therefore strongly linked to volume changes 344 associated with metamorphic reactions.

345 Figure 6b displays the value of $\Delta \tau$ as a function of *P* and $\dot{\varepsilon}$ for dry anorthite (Rybacki and Dresen,

346 2000). $\Delta \tau$ isocontours are presented in black. The brittle-ductile transition (BDT, yellow line) corresponds to $\Delta \tau = 0$. Conditions of the parametric study performed for different degrees of 347 348 overstepping (right vertical axis) and different background strain rates considering a density difference $\Delta \rho$ of 400 kg.m⁻³ (i.e., roughly as in the granulite to eclogite transformation) are also 349 350 presented (see symbols). White lines correspond to isovalues of the amount of anorthite matrix that 351 undergone brittle failure in case of reaction-induced volume change. An illustration of the effect of 352 the background strain rate is presented in Fig. 6c-g. Results show that the field where yield stress is 353 achievable due to reaction-induced volume change covers a large part of the domain where ductile 354 deformation is expected for dry anorthite if metamorphic transformation were not activated (Fig. 355 6b). By accounting for the stress induced by volume change, the position of the brittle-ductile 356 boundary can be shifted towards lower strain rate values, reducing the required strain rate necessary 357 to fail the rock up to two orders of magnitude. Destabilization of a ductile metastable granulite into 358 eclogite anywhere in this domain can lead to brittle failure.

4. Discussion and conclusion

360 Our results show that eclogitization-induced densification occurring under metastable conditions 361 can, by itself, generate sufficient shear stress to fail the rocks at high-pressure conditions. Brittle 362 failure in rocks can therefore be explained by densification reactions, without even considering the rheological changes induced by the reaction. In light of these results, it is now possible to further 363 364 discuss the applicability of our model on natural cases and the broader implications of this study on 365 the strength of the continental lithosphere subjected to metamorphic reactions. These points will be 366 addressed in the following, after a discussion on possible perspectives concerning our modelling 367 approach.

368 **4.1. Modelling perspectives**

369 In the present study we intentionally did not consider the potential rheological changes associated 370 with the metamorphic transformation. Modification of strength is transient and only caused by 371 densification. This choice has been made to isolate and study in detail the effect of densification alone. One important consequence of this is the value of pressure obtained in the transforming area, 372 373 which is lower than the pressure in the unreacted matrix. However, in models considering only 374 strength difference between inclusion and matrix (as in Fig. 5c, d), the weaker the inclusion is 375 compared to its matrix, the higher the pressure difference will be between the inclusion and matrix (Schmid and Podladchikov, 2003; Moulas et al., 2014, Luisier et al., 2019). We can therefore 376 377 speculate that by taking into account a viscosity decrease of the inclusion in addition to volume 378 change during the transformation would lead to higher pressure inside the inclusion compared to 379 models that only consider volume changes. Depending on the magnitude of such a viscosity 380 decrease, the pressure inside the inclusion could even be higher than the pressure in the surrounding 381 matrix. In such a case, this pressure increase would extend the degree of overstepping of the rock. 382 This is something that can be expected for the eclogitization process in specific cases, such as the granulite to eclogite transformation, as it is classically proposed that the eclogite is weaker, at least 383 transiently, than its granulitic protolith (Labrousse et al., 2010; Bras et al., 2021; Kaatz et al., 2021). 384

Our models assume that the third direction of space is infinite. Our analytical solution (see section 2.2) shows that the stresses induced by volume change ("self-induced stresses") in cylindrical coordinates corresponds to 2/3 of the self-induced stresses obtain in spherical coordinates (Lee and Tromp, 1995; Gillet et al., 1984). Hence, considering the eclogitization process in 3D would therefore lead to higher self-induced stresses than in 2D. In that sense, our estimates of the ability to reach brittle failure can then be taken as minimum.

We assume conservation of mass and thus consider a closed system. A variation of density therefore only impacts volume change. However, it is well known that any replacement reaction, whether it is a volume increase or reduction, involves the formation of intra-crystalline porosity along with the product minerals, as evidenced by pseudomorph microtextures (Putnis, 2002; 2009; 2015). In the case of an open system subjected to input of externally derived fluids, such a porosity can be filled by product minerals, thus limiting or even inhibiting the volume change (Centrella et al., 2015). 397 Similarly, mineral replacement can occur via a process of isovolumetric interface-coupled
398 dissolution-precipitation during open system fluid-rock interaction (Putnis, 2009; Centrella et al.,
399 2015). From this point of view, our model constitutes an end-member that can however be applied
400 in cases where mass balance is fulfilled (Centrella et al., 2018).

401 **4.2. Applications and Implications**

402 The degree of overstepping a rock can sustain before reacting plays a major role on its mechanical 403 behaviour. Indeed, our results show that it extends the brittle field toward lower strain rate values 404 (Fig. 6). Many examples have been reported where the plagioclase breakdown reaction is thought to 405 have been inhibited because of the lack of free fluid (Austrheim, 1987; Wayte et al., 1989; Rubie, 406 1998; Jackson et al., 2004; Young and Kylander-Clark, 2015; Jamtveit et al., 2016; Palin et al., 407 2017). The preservation of metastable plagioclase at high pressure can generate pressure 408 overstepping of the order of several 100's of MPa as already suggested by Wayte et al. (1989) for 409 the Allalin metagabbro (Alps) and Hetényi et al. (2007; 2021) for the Indian lower crust (beneath 410 the Tibetan Plateau), and sometimes up to pressure higher than 1.0 GPa (e.g., Wain et al., 2001). 411 Densification of rocks triggered by mineral reactions that take place far from the equilibrium constitutes therefore a mechanism for explaining the nucleation of mechanical instabilities at depth 412 413 during the burial of a dry continental lithosphere and it is in good agreement with kinetics laws (e.g. 414 Cahn, 1956). In the case of a densification reaction such as the eclogitization of plagioclase-bearing 415 rocks (e.g. Norvegian or Himalayan granulites, Alpine gabbros), it is hence appropriate to study the 416 effects of volume change on the initiation of such instabilities.

417 Assessing the seismic potential of such a failure occurring at intermediate depth in continental 418 subduction zones is challenging and remains under the scope of this study. The question regarding 419 their potential seismogenic nature remains open and could be answered by using dynamic rupture 420 models (Gabriel et al., 2020, Thomas and Bhat, 2018) and/or laboratory experiments (Schubnel et 421 al., 2013).

422 Our results also show that the mechanical effect of reaction-induced volume change on deformation is important even if only a small amount of material is transformed. Reaction-induced shear stress is 423 424 indeed maximum when the initial amount of material allowed to react is small (<10%, see Fig. 4b). 425 Maximum shear stress values then gently decrease when the ratio between the initial volume of 426 reacting material and total volume of rocks increase (Vol_{inc}/Vol_{tot} in Fig. 4b), reaching a plateau of low shear stresses for values of Vol_{inc}/Vol_{tot} ~30-40%. This is in good agreement with the absence 427 428 of seismicity observed in subducting continental crust where eclogitization progress exceed 30-40% 429 (see Fig. 1a, b). This could explain why pseudotachylytes are only observed in partially transformed 430 granulites from Holsnøy (Fig. 1d-f), where the percentage of eclogitization is below ~40% (Boundy 431 et al., 1992).

432 In addition, our results show that even if frictional yielding is reached, the amount of material that 433 undergoes plastic deformation is generally low (i.e., in the order of 1% or less, see Fig. 6). 434 However, this should not be overlooked. When yielding occurs, the pressure in the damaged area 435 drops. In contrast, pressure increases at the tip of the area that has undergone plastic deformation 436 (Fig. 5b). The development of such a pressure gradient could be responsible for a transfer of fluid that may favourably circulate through the damaged zone. Because transformation of granulite into 437 438 eclogite is mainly driven by the presence of fluids, we can speculate that, if even a small amount of 439 fluid is present in the granulite, it will favourably be collected toward the damage zone and then allow transformation of this area. Figure 7 displays a model where this hypothesis is tested, by 440 441 allowing areas that have undergone plastic deformation to react (i.e., by allowing density change as 442 it is the case for the initial reacting inclusion). It illustrates progressive eclogitization by a runaway 443 mechanism, which lasts as long as the reaction is not limited by the lack of reactive product. In that 444 case, eclogitization of the granulite self-propagates in the direction perpendicular to the shortening direction, forming finger-like structure of eclogitized material as described in the Holsnøy area 445 446 (e.g., so-called "static eclogites", Putnis, 2021; Zertani et al., 2019, Jamtveit et al., 2000; 2016).

447 This study has therefore strong implications for our understanding of the state of stress of the

448 continental lithosphere in convergence zones. In such geodynamic contexts, rocks buried at depth 449 are mainly subjected to metamorphic reactions leading to an increase in density. Our results show 450 that the nucleation of brittle instabilities due to the densification reaction taking place far from 451 equilibrium can generate important transient stresses, hence extending the domain where frictional 452 plastic yielding can occur.

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656				
657	Data availability			
658	All numerical model outputs are available from the corresponding author upon request. They can			
659	also be reproduced by using the scripts provided in supplementary materials.			
660	Code availability			
660 661	Code availability Matlab scripts for the analytical solution and the 1D model are provided in supplementary			
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- 671 The authors declare that they have no known competing financial interests or personal relationships
- that could have appeared to influence the work reported in this paper.

Table 1 Parameters used in reference models

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n	1	1	
v			

Symbol	Meaning	Unit	Value				
1D reference model (without background strain rate and using linear viscosity)							
$P_{\rm BG}$	Background pressure	GPa	2.0				
Pr	Pressure of reaction	GPa	1.5				
$\Delta P_{\rm m}$	Pressure overstepping (P _{BG} -P _r)	GPa	0.5				
<i>d</i> _{Pr}	P _r standard deviation	GPa	0.7				
$ ho_1$	Initial density (before transformation)	kg.m⁻³	2850				
ρ_2	Final density (after total transformation)	kg.m⁻³	3250				
<i>t</i> _k	Kinetic parameter*	S	3.1558×10 ⁹				
K	Bulk modulus	GPa	80				
G	Shear modulus	GPa	40				
η	Viscosity	Pa.s	10 ²²				
2D reference model (with background strain rate and visco-elasto-plastic rheologies)**							
έ _{BG}	Background strain rate	S	10-14				
T_{BG}	Temperature	°C	680				
A	Pre-exponential factor (dislocation creep)***	Pa ⁻ ".s⁻'	5.0119×10 ⁻ °				
n	Exponent (dislocation creep)***	-	3				
Ea	Activation energy (dislocation creep)***	kJ.mol⁻¹	648				
С	Cohesion	MPa	50				
arphi	Friction angle	0	30				
$\eta_{ m vp}$	Viscoplastic viscosity	Pa.s	5 ×10 ¹⁸				
$C_{ m p}$	Heat capacity	J.kg⁻¹.K⁻¹	1050				
k	Conductivity	W.m ⁻¹ .K ⁻¹	2.3				

*see Supplementary Fig. 1 for more details **Parameters that are the same in both 1D and 2D model (i.e. elastic and metamorphic reaction properties) are not recalled for 2D reference model. ***Values from Rybacki and Dresen (2000) for anorthite dry.

- 679 **Figures and captions:**
- 680 **Figure 1**



682 Fig. 1 (a) Cross-section in southern Tibet with seismicity datasets from Monsalve et al. 2006, Monsalve et al. 683 2009 and Schulte-Pelkum et al. 2019. Seismic events in the upper crust are plotted in grey. Deeper events are 684 in black. Abbreviations: U.C. = upper crust, L.C. = lower crust, MBT = Main boundary thrust, MCT = Main 685 Central Thrust, STD = Southern Tibet Detachment, YTS = Yarlung Tsangpo Suture, MHT = Main 686 Himalayan thrust. (b) Estimated amount of eclogitization of the lower crust for the same cross-section (after 687 Hetényi et al., 2007; 2021 and Schulte-Pelkum et al., 2005). c, d, e: Field photographs from Holsnøy 688 displaying progressive eclogitisation of lower continental granulite. (c) Untransformed granulite mainly 689 constituted by garnet, plagioclase and pyroxene (red, white and black minerals, respectively). (d) High-690 pressure pseudotachylyte formed during eclogitization (Austrheim and Boundy, 1994; Bjørnerud and

- 691 Magloughlin, 2004). (e) Granulite fully transformed into eclogite with garnet (red), omphacite (green) and
- 692 zoisite-kyanite-quartz (yellowish assemblage). (f) Possible evolution of rock's density with pressure during
- the granulite to eclogite metamorphic transformation. Black stars correspond to density data extracted from
- 694 Perple_X_6.9.1 (Connolly, 1990; 2009) at $T = 680^{\circ}$ C (see details in section 2.5.). Blue curve corresponds to
- 695 a possible fit of the density evolution using a cumulative distribution function with a mean pressure (P_r) of
- 696 1.35 GPa and a standard deviation (d_{Pr}) of 0.7 GPa as defined in Fig. 2b and considering reference densities
- 697 of 2850 kg.m⁻³ and 3290 kg.m⁻³ for granulite and eclogite, respectively.



703 Fig. 2 (a) Pressure (P) – temperature (T) diagram presenting a metamorphic reaction (orange line) associated 704 with a density change (from ρ_1 to ρ_2). ΔP_m corresponds to the initial pressure overstepping, i.e. the difference 705 between the background pressure (P_{BG}) and the pressure of the metamorphic reaction (P_r) , for a fixed 706 temperature. (b) Model of density evolution of a rock in thermodynamic equilibrium along the pressure path 707 of Fig 2a. (dashed line). This model (blue line) corresponds to a cumulative distribution function centred on 708 P_r with a standard deviation of d_{Pr} that controls the density change sharpness. It also reflects the progress of 709 the reaction from X = 0 (unreacted material) to X = 1 (fully reacted material). (c) 1D model setup (see section 710 2.3). L is the total length of the model. r_{inc} is the part where metamorphic reaction (i.e. density change) 711 occurs. (d) 2D model setup with background strain rate ($\dot{\epsilon}_{BG}$) as boundary conditions (dark blue arrows, see 712 section 2.4). Green inclusion (reacting area) has the same material properties as the matrix, but density 713 change associated with metamorphic reaction is activated in this domain.



717 Fig. 3 Evolution of shear stress (a-c), pressure and velocity field (d-f) for the 2D reference model with time 718 (top-right quarter of the model only). Parameters used are those of the 1D reference model (see Table 1). For 719 comparison, results from the 1D model (see section 2.3. and Table 1 for parameters) are presented in (g) to 720 (i) as follows: (g) Evolution of pressure with reaction progress (X) in matrix (black line) and in the reacting 721 area (green line). Circle, asterisk, plus and multiplication symbols corresponds to different times (0.5, 10, 50, 722 100 and 250 kyrs, respectively). Blue line is for a rock in thermodynamic equilibrium. (h) Evolution of 723 pressure with time (t) for matrix (black line) and reacting area (green line). (i) Evolution with time of 724 maximum of shear stress $(max(\tau_{II}))$ recorded in the matrix.

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727 **Figure 4**





Fig. 4 Shear stress generated by volume change. (a) Colourplot of maximum of shear stress, max(τ_{II}), recorded in the matrix as a function of degree of overstepping (ΔP_{m}) and density change associated to the metamorphic reaction ($\Delta \rho$). White dots correspond to the reference models presented in Fig. 3 (peak of max(τ_{II}) in Fig. 3i). (b) Influence of the initial size of the reacting area on the obtained maximum shear stress. Red star corresponds to result obtained in reference model (i.e. with $r_{inc} = 0.25$ m and L = 2 m). Vol_{inc}/Vol_{tot} = $\pi r_{inc}^2/L^2$.

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739 Fig. 5 Volume change vs. viscosity contrast under pure shear deformation. Results are extracted from the 2D model (see section 2.4. and Table 1 for parameters) at $P_{BG} = 2$ GPa , $T = 680^{\circ}$ C and $\dot{\varepsilon}_{BG} = 10^{-14}$ s⁻¹ after t =740 741 500 yrs. Each plot displays two panels as follows: (top) pressure field (bottom) shear stress (i.e. second 742 invariant of the stress tensor) field. Plasticity is switched-off for models (a) and (c) and activated for models (b) and (d). In (a) and (b), densification is activated in the reacting inclusion ($\Delta \rho = 400 \text{ kg.m}^{-3}$; $P_r = 1.5 \text{ GPa}$; 743 744 $d_{\rm Pr} = 700$ MPa) but inclusion and matrix have the same material property (Table 1). Viscosity present a stress 745 exponent (n=3). In contrast, in (c) and (d), volume change due to the reaction is switched-off and the only 746 difference between the inclusion and the matrix corresponds to a viscosity ratio (reference viscosity in the 747 inclusion is 10^3 times weaker than in the matrix, and n=3). White contours delimitate the parts of the matrix 748 that reached the yield stress and have undergone brittle failure.



754 Fig. 6 Overstepping and strain rate effects on brittle-ductile transition. (a) Loading curves for a visco-elasto-755 plastic material undergoing ductile deformation (in blue) and frictional deformation (in green). $\Delta \tau$ is the 756 difference of shear stress (τ_{II}) between τ_{v} (yield stress value) and τ_{v} (viscous shear stress). (b) Values of $\Delta \tau$ in 757 the P vs. $\dot{\varepsilon}$ diagram for anorthite dry (see parameters in Table 1) at $T = 680^{\circ}$ C. Symbols correspond to 758 simulations performed using the 2D model (see section 2.4.) at $T = 680^{\circ}$ C for $P_r = 1.5$ GPa and $d_{Pr} = 700$ 759 MPa. Results (extracted after t = 1000 yrs) allows to define the ratio between the amount of matrix area that reached the yield stress (A_{brittle} , red colours in (c-g)) and the total amount of matrix material (A_{matrix}). Areas 760 depicted in orange and red correspond to zones that reached a plastic strain of 10⁻⁵ and 10⁻³, respectively. 761 762 White dashed lines in (b) correspond to isocontours of this ratio (in %). BDT = Brittle-ductile transition. Five 763 different symbols are used to group the similar results: Grey dots are used for models similar to (c), i.e. 764 where brittle features are not significant; + signs are used for models as in (d) and (e), x signs are used when 765 shear zones start to propagate as in (f); stars are used when well developed shear zones propagate as in (g); 766 red stars correspond to models belonging to the brittle domain as illustrated in Supplementary Figure 5.

768 **Figure 7**



Fig. 7 Models of transformation propagation. In these models, the parts of the matrix that reached an accumulated plastic strain of 10^{-3} (i.e., red area from Fig.6e) are allowed to react (i.e. same properties as the initial inclusion are affected to them). (a) Reaction progress with time (b) Pressure evolution. Black contour corresponds to the initial position of the reacting area. White line shows the orientation of the maximum principal stress (σ_1) applied on the model.

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