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Effect of phase transitions on seismic properties of metapelites: a new high-temperature laboratory calibration

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ABSTRACT

We report new measurements of the seismic properties of an upper amphibolite facies metapelite from the Serie dei Laghi basement (Southern Alps, N-Italy), presenting evidence for the α-β transition using elastic wave velocity methods and under in situ conditions. Measurements were made using an internally heated gas apparatus under hydrostatic conditions to 500 MPa and temperatures to 1075 K. P-wave and S-wave velocities were measured parallel and normal to both lineation and foliation at room temperature. An average V_p (at 400 MPa) of 6.4 km/s and V_p anisotropy of 15% were found and an average Vs_1 of 3.6 km/s (8.2% anisotropy), and Vs_2 of 3.5 km/s (4.1% anisotropy) were also measured. To observe the effects of the α-β quartz transition under hydrostatic conditions, elastic wave velocity was monitored continuously as the sample was heated to 1075 K. At 400 MPa, V_p was seen to decrease monotonically with temperature to 950 K; as temperature continued to increase V_p rapidly increased until 1075 K. The effect was found to be reversible and is interpreted in terms of the α-

β transition in quartz, in broad agreement with previous studies. A simple interpretation of the data, taking into account a field case example from southern Tuscany as well as natural and elevated geothermal gradient suggests that thermal and hydraulically driven fracture is a likely cause of 'bright spots' seen in these areas. With knowledge of the depth of such features, the transition additionally allows the temperature at depth to be estimated.

INTRODUCTION

Phase transitions are a common phenomenon in all materials, including geological minerals. Of these minerals, arguably the most important in crustal rock forming processes is quartz, whose phase change between its alpha (α) and beta (β) types was first discovered by Le Chatelier (1889) at temperatures above 846 K. This phase transition is accompanied by a change in symmetry, volume, and shape, with the higher temperature β-phase possessing a higher symmetry and larger volume than the α-phase. The critical temperature, T_c, at which this transition occurs is also known to be a function of pressure. Theoretical thermodynamic calculations show that T_c is linear with increasing pressure (Majumdar et al., 1964; Coe and Paterson, 1969) up to the pressure of the quartz–coesite reaction. At 400 MPa, the T_c is at 946 K, corresponding to conditions found at a depth of ~16 km and 30 km respectively when considering solely the lithostatic and geothermal gradient.

Because of the pronounced increase in P-wave elastic wave velocity (v_p), due to the change in symmetry and volume, the α-β transition in quartz has been previously proposed as a thermometer for depth (e.g., Mainprice and Casey, 1990; Mechie et al., 2004) when combined with knowledge of the linear T_c / P relationship. However, there are relatively few experimental studies of the α-β transition in quartz-rich rocks, with only the experiments of Kern (1979, 1982) and Kern and Richter (1981) reporting the transition in three quartz rich samples (a quartzite, a granite and a granulite) at pressures up to ~300 MPa. Well-calibrated data relating the P-wave velocity to pressure and temperature on other lithologies more representative of the middle crust, such as metapelites, are therefore key to using this method as a diagnostic tool for determining temperature conditions at depth.

Although the temperatures required are above those expected from the natural geothermal gradient, there are areas where it has been demonstrated that the high heat flux has resulted in anomalous seismic recordings, subsequently interpreted as evidence for the α-β transition (Marini and Manzella, 2005). To explore these effects, and to better calibrate the role of pressure and temperature on the phase transition as measured by elastic wave velocity, we report an experimental study in which we have performed a number of hydrostatic tests on a quartz rich metapelite rock up to temperatures of 1050 K, well above the expected α-β transition.

SAMPLE MATERIAL AND EXPERIMENTAL METHODS

Geological Setting and Sample Preparation

For the experiments, we chose a quartz rich metapelite from the Kinzigite Formation of the Ivrea-Verbano Zone (south alpine domain, northern Italy). The Ivrea-Verbano comprises a metapelitic sequence (known as the Kinzigite Formation) together with a large Mafic Complex, and with numerous lenses of ultramafic rocks (spinel peridotites). The Kinzigite Formation consists of amphibolite to granulite facies metasediments, with interlayered metabasites, quartzites and incorporating thin metacarbonate horizons. The area is widely considered to represent an exhumed crust-mantle transition (Fountain, 1976; Zingg, 1983) on the strength of the presence of spinel lehrzolite lenses in the granulites near the mafic intrusion. The samples were typical metapelites equilibrated under upper amphibolite conditions, visually free from weathering, and with only very localized traces of retrograde metamorphism along microfractures. Sillimanite (fibrolite) was observed in small needles elongated parallel to the lineation, but in insufficient quantities and with a grain size too small to determine lineation. The modal composition, determined via scanning electron microscopy through analysis of the back-scattered image, is Quartz 36.5%, Plagioclase 34.1%, Biotite 14.3%, Muscovite 10.7%, Chlorite 3.3% and secondary mineals 1.0%.

Right cylindrical cores were prepared of 25.4 mm and 22 mm diameter for room and high temperature measurements respectively, and of 30 mm length. Samples were drilled along three mutually orthogonal directions in order to determine seismic wave velocity anisotropy. It is well known that anisotropy in both P-wave (V_p) and S-wave (V_s) velocities is disproportionally effected by the alignment of microstructure and microcracks (e.g., Benson et al., 2006), and therefore a-priori knowledge of this anisotropy is important for later interpretation. The observed foliation and the lineation of the pelite denote the reference frame. We define 'X' cores parallel to the lineation, 'Z' cores normal to the foliation, and 'Y' cores normal to the lineation and parallel to the foliation (see insert in Fig. 1). Faces of the cores are polished parallel to within 0.02 mm, and oven dried for 24 h at 80 °C.

Methods

The compressional (V_p) and shear (V_s) elastic wave velocities were measured using the pulse transmission technique (Birch, 1960) at temperatures up to 1023 K and pressures up to 450 MPa using an internally heated gas medium apparatus equipped with a hybrid waveguide and embedded piezoelectric elements (PZT) to transmit and receive waveforms through the sample. Detail of the experimental setup are reported in Burlini et al. (2005) and Burlini et al. (2007). The length of specimens were measured before and after each experimental run so as to ensure errors introduced via sample length change were minimised All velocity measurements were made at a frequency of 1 MHz. We estimate uncertainties of ~0.7% for V_p, 1.5% for V_s, and 1K for absolute temperature.

Compressional and shear wave velocities were measured simultaneously via a dual PZT transducer arrangement. V_p and V_s were measured at intervals of 50 MPa in confinement up to a maximum of 450 MPa, with the same intervals during decompression. In order to avoid thermal cracking of the samples, a specific experimental protocol was adopted. After an initial confining pressure was applied, both pressure and temperature were increased at steps of 100 MPa and 100 K respectively until 400 MPa and 773 K was reached, with decreasing pressure made in steps of 50 MPa and 100 K. In subsequent runs, pressure and temperature were simultaneously increased up to the previously attained values, at which point the pressure was maintained at 400 MPa while temperature was increased on its own in steps of ~20 K up to the maximum temperature of 1023 K. Using this specific PT path we avoided thermally overly-stressing the samples at low confining pressure, which were recovered intact after the tests. Experiments at high pressure and temperature were made on samples (Z) drilled perpendicular to foliation, and (X), parallel to lineation, with a focus on the key temperature range of 943 K to 1023 K, where we expected the phase transition to occur, in order to maximise resolution via a more detailed curve of 10K steps, and at pressures from 200 to 400 MPa. Only V_p data were recorded during these runs.

RESULTS

Seismic Properties at Room Temperature and Elevated Pressure

Figure 1 shows elastic wave velocity with increasing pressure under room temperature conditions. V_p (Fig. 1A,) increases with pressure, with the bulk of the increase accommodated at pressures less than 150 MPa, after which the increase becomes essentially linear with pressure. This is a well known rock physics effect, with the nonlinear part of the curve attributed to crack and pore closure, and the linear segment expressing the intrinsic properties of the rock (Birch, 1961). As the pressure increases, the coefficient of anisotropy, defined as A = 100% * (V_{max}-V_{min}) / V_{mean} where V_{mean} is (V_x+V_y+V_z)/3 initially increases, and then decreases rapidly from a maximum of nearly 25% to a quasi steady-state value of 14% (solid line, Fig. 1A). While we do not make the multiple directional measurements strictly needed for the definition of the full velocity anisotropy tensor (e.g., Benson et al., 2005), knowledge of the fabric alignment and how these microstructures effects elastic wave anisotropy suggests that the maximum anisotropy is well described by the cores taken in the X, Y and Z direction (e.g., Benson et al., 2006).

The situation for S-wave elastic data is complicated by the polarization of the wave with respect to the fabric of the sample. As well as the anisotropy with respect to the propagation direction, the shear wave splitting (birefringence) is also prominent as a result of the fabric of the metapelites, which contain minerals such as mica. In figure 1B, we show S-wave elastic data in the same three principal directions, denoted V_s [x], V_s [y] and V_s [z], but with polarization orientated in either the XY or XZ planes for 'X' axis cores, XY or YZ planes for 'Y' axis cores, and the XZ or YZ planes in the case of propagation along the axis of 'Z' axis cores (inset, Fig. 1A). For 'X' axis cores, V_s increases from 3.28 and 3.35 km/s at low pressures to 3.57 and 3.70 km/s at 500 MPa for the two polarisations respectively. For 'Y' axis cores, the V_s [y] trend is similar, although with a slower increase over the first 200 MPa. Finally, V_s [z] data have the lowest velocities, ranging from 3.06 km/s to 3.45 km/s at 500 MPa.

We note that the polarization velocities are self-consistent at high pressures (above ~400 MPa), V_s polarized in the foliation has a higher velocity than polarized normal to foliation for both the X and Y directions, with similar values for both V_s[y] and V_s[x] (Fig. 1B). This suggests that lattice preferred orientation (LPO) of the minerals is the key control on the S-wave velocity in this metapelite. Further evidence of the complexity relating to the LPO, intrinsic and extrinsic effects, and S-wave velocity propagation direction can be seen from the velocity path as pressure is increased. The V_s[x] velocity increases more quickly than the V_s[y] velocities, an effect that can be attributed to the [x] direction being more closely aligned parallel to the foliation orientation than the [y] direction. V_s measurements in this direction are likely to take into account a higher proportion of raypaths cutting across the foliation plane resulting in a slower Vs increase with pressure. However, the eventual convergence of the velocities at ~350 MPa implies that all cracks and extrinsic effects are insignificant by this pressure.

Seismic Properties at Elevated Temperature and Pressure

After the initial measurements described above, a subset of samples was selected for determining the V_p response of the metapelite to high temperatures, up to and beyond the expected α-β transition. Samples were heated up to 1020 K at 400 MPa (Fig. 2). As temperature was increased, V_p decreased from ~7 km/s to 6.6 km/s at ~950 K (open and close diamonds denoting measurement with increasing and decreasing temperature, respectively, along the X propagation direction). After this point, P-wave velocity increases to 7 km/s at ~1000 K. For samples orientated in the Z direction, a similar pattern was obtained.

Once the general location of the transition was established, a further set of experiments was performed in order to locate it more precisely as a function of temperature at three different pressures (Fig. 3). At each pressure, a similar velocity minimum was observed. However, this minimum value progressively moved to higher temperatures as pressure was increased. We recorded a minimum V_p of 6.05 km/s at 890 K (200 MPa), 6.15 km/s at 920 K (300 MPa), and 6.325 km/s at 950 K (400 MPa). Assuming a linear fit, this yields 4.6 m/s rise in V_p per 1 K increase in temperature, or a rise of 3.3 MPa per 1 K. Alternatively, the expressions can be combined to give an increase of 1.4 m/s per 1 MPa increase in pressure, that can be linked to the lithostatic pressure gradient.

DISCUSSION AND CONCLUSIONS

The α-β transition, although known and understood for many decades (e.g., Coe and Peterson, 1969; Van der Molen, 1981; Kern, 1982), is a likely candidate for a number of more recent observations such as seismic bright spots observed at depth in geothermal areas (Marini and Manzella, 2005) due to the abnormally high heat flux in such areas. The volume associated with the phase change of the quartz has the secondary effect of fracturing the surrounding minerals through a process essentially analogous to thermal stressing (e.g., Vinciguerra et al., 2005) and thus leading to locally different physical properties. As the transition occurs at precise conditions of pressure and temperature, the effect could, in principle, be used as a marker of temperature when observing diagnostic seismic effects such as abnormal reflections, especially in areas of higher than average geothermal gradient. As P-wave data are more greatly affected by the transition compared to V_s (Kern, 1982), our experiments concentrated on V_p as a function of increasing pressure and at three key temperature ranges (Fig. 3).

An interpretation of these data can be made either in terms of the changing V_p value with pressure, and therefore the equivalent depth in the lithosphere, or as a relationship between the temperature and either velocity (at known pressure) or a pressure (given an assumed temperature). Our sample is hydrostatic thermodynamic equilibrium, thus the V_p velocity minimum (Fig.3) corresponds to the α-β transition temperature at pressure and temperature of the experiment. Shen et al. (1993) provides an accurate experimental determination of the transition temperature using laser interferometry. At 200, 300 and 400 MPa Shen et al. (1993) calibration gives the temperatures 899.22, 923.49 and 948.64 K, whereas from Fig.3 the observed Vp minima are 890, 925 and 950 K. This excellent agreement allow us to consider our system in hydrostatic thermodynamic equilibrium with a high level of confidence. Given that the temperatures are likely to be higher than the standard geotherm (~22.1 K/km) such transitions are to be detected via seismic methods, then it is logical to discuss the ability of this phenomenon to act as a temperature probe at depth if the velocity of the unit can be measured at an assumed depth. Figure 4 shows the results of this interpretation, in which the measured P-T relationship have been plotted together with a standard geotherm. To use the transition as a diagnostic tool data combining the known transition and the depth to a target horizon can, in concept, be used to infer the local temperature given the measured 7.5 K/km increase with depth from our laboratory investigation. Simultaneously, the measured V_p at the transition temperature increases by ~30 m/s per km. Finally, a relationship between P-wave velocity and temperature can also be established, yielding an increase 4.6 m/s per K rise in temperature. However, it must be noted that this relationship is driven by the pressure increase with depth and therefore cannot be used directly.

The most effective way to employ the α-β transition as a probe for temperature is to first establish the depth of interest. Previous studies have employed seismic reflection data to identify a target anomaly known as the K horizon (Marini and Manzella, 2005). As this depth (between 5 and 6 km, 125–150 MPa), one can use the laboratory calibrated data to infer the likely temperature expected for the transition, ~880 K, and the associated P-wave velocity, ~6 km/s. Although this presents something of a circular argument, this approach nonetheless results in a P-wave value which is not inconsistent with the P-wave velocity derived from the seismic data processing. In other areas the K horizon lies deeper at 10–12 km (Cameli et al., 1998; Liotta and Ranalli, 1999) where the corresponding α-β transition lies at ~920 K and 6.1–6.2 km/s.

In areas of high heat flux (124 K/km in the example of Southern Tuscany, Marini and Manzella, 2005), local temperature can increase to an extent whereby quartz undergoes its phase change under pressures that permit deformation in the brittle regime. Under such conditions, fracturing of the surrounding minerals is likely, the conclusion reached by Marini and Manzella (2005). In this case a 'bright spot' in the seismic section is interpreted as the influence of high impedance fluids filling up the spaces created by fracturing driven by the α-β transition. Outside areas with high geothermal gradient, the depth required before the α-β transition would be encountered is much higher, at ~36 km. However, at these depths the deformation of the crust lies in the ductile regime and therefore the increase in volume is unlikely to lead to the fracturing of surrounding minerals, and therefore the detection of the transition using seismic reflection methods would not be possible, likely explaining the lack of such data at this depth.

In this study we have re-visited the phenomenon of the α-β transition in quartz, extending the conditions of experimental investigation to a wider pressure range over those previously published by Kern (1982) and analyzing a rock that is representative of the middle continental crust (metapelite). We measure V_p and V_s data continuously over set pressures up to 500 MPa and, for V_p, over a continuously varying temperature range to map the α-β transition in detail. We have found that the transition temperature occurs at the same temperature regardless of the orientation at which the sample is measured (Fig. 1), but that the sharpness of the V_p trend is affected by the anisotropy of the sample, leading us to draw the conclusion that the variation has a sensitivity to the anisotropy and crystallographic orientation. There is an increase in the transition temperature of ~0.3 K/MPa, consistent with previous experimental petrological determinations of the alpha beta transition (Shen et al., 1993) and with the previous numerical calculations of Johnson et al. (1992), or 7.5K per km depth in the lithosphere assuming a density of 2.5 g/cm^3. In areas of high heat flux it is likely that quartz rich rocks may undergo the transition at shallow levels (5–6 km, equivalent to 893–1017 K), resulting in the higher volume β phase fracturing the surrounding minerals in the brittle regime. We measured a linear trend of the transition with both temperature and P-wave velocity as a function of pressure. Taken together, this allows areas in which abnormally high geothermal gradient to be interpreted in terms of their temperature profile by tracking the α-β transition through shallow, local, fracturing produced by thermal cracking with a high level of confidence.

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FIGURE CAPTIONS

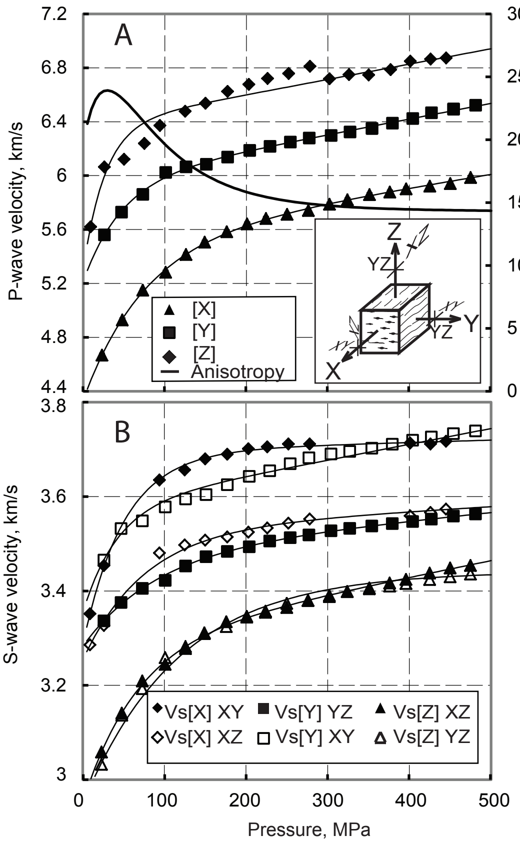
Figure 1. Effect of pressure at room temperature on P–wave velocities. The P wave velocities measured along the three structural direction: X parallel to lineation; Y normal to lineation and parallel to foliation; Z normal to foliation, (insert) are plotted in panel A. Six shear-wave velocities are reported in panel B, using shear wave notation similar to stress-strain notation: the

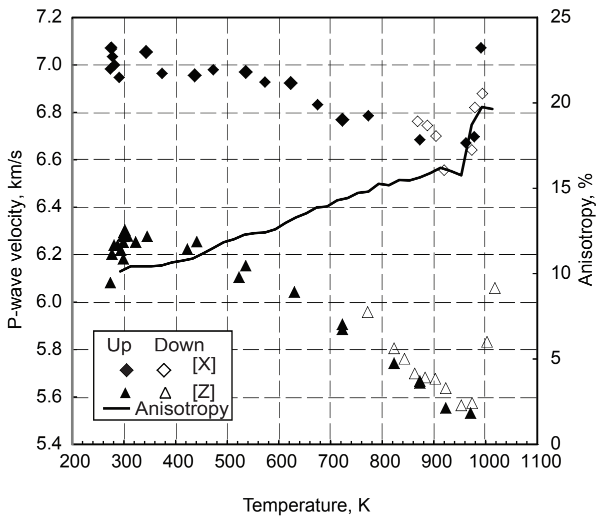
first index indicates the direction of particle motion and the second the direction of wave propagation (insert). Elastic wave velocities are fit to the equation after Wepfer and Christensen (1990).

Figure 2. Change of P-wave elastic velocity as a function of temperature, at 400 MPa confinement, for two cores parallel (X) and normal(Z) to the foliation direction, with increasing (open symbol) and decreasing (closed symbol) temperature. In each case a clear minimum is observed due to the α–β transition, accompanied by a decrease in the anisotropy (solid line).

Figure 3. Detail for the velocity change over the transition for metapelite studies, for 200, 300 and 400 MPa pressure.

Figure 4. Interpretation of the temperature increase expected from the increasing pressure at dept for the α–β transition (dashed line, with circles denoting data points), as compared to the standard geothermal gradient (solid line) on stable cratons. In areas of highheat flux, the transition will occur at depths much smaller than expected due to the standard geotherm (~36 km).


A
B
P-wave velocity, km/s
Anisotropy %
S-wave velocity, km/s
Pressure, MPa
[X]
[Y]
[Z]
Anisotropy
Z
YZ
Y
X
Vs[X] XY
Vs[Y] YZ
Vs[Z] XZ
Vs[X] XZ
Vs[Y] XY
Vs[Z] YZ


P-wave velocity, km/s
Anisotropy, %
Temperature, K
Up
Down
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Anisotropy
7.2
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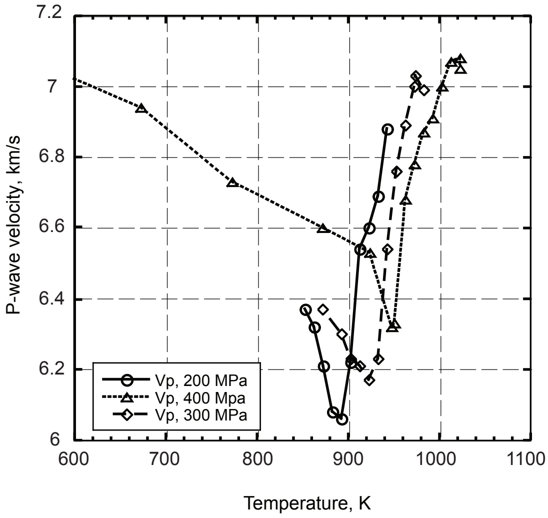
7.2
7
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6
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1000
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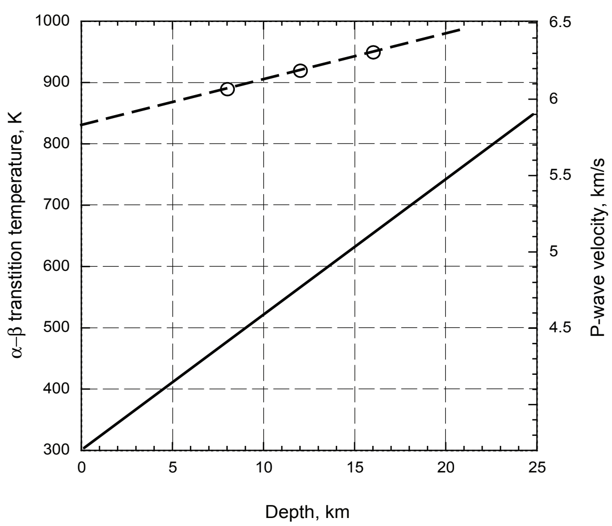
P-wave velocity, km/s
Temperature, K
Vp, 200 MPa
Vp, 400 Mpa
Vp, 300 MPa



α–β transtition temperature, K
P-wave velocity, km/s
Depth, km
1000
900
800
700
600
500
400
300
6.5
6
5.5
5
4.5
0
5
10
15
20
25