Seismic Signature of the Continental Crust: What Thermodynamics Says. An Example From the Italian Peninsula

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Abstract

Unraveling the temperature distribution and composition of Earth’s crust is key for understanding its origin, evolution, and mechanical behavior. Models of compressional ($V_p$) and shear wave ($V_s$) velocity are obtained from seismological studies and can be interpreted in terms of temperature and composition, using relationship defined through laboratory experiments. These empirical evidences often do not properly account for the effects driven by temperature, pressure, water content, and phase change of minerals. In this study, we use thermodynamic modeling to properly investigate the role of these variables in affecting seismic properties, as a tool to guide (joint) inversion and interpretation of geophysical data. We find that mineralogical phase transitions can be more seismically relevant than a change in chemical composition. In particular, the $\alpha-\beta$ quartz transition would cause a jump in acoustic impedance and $V_p/V_s$ ratio $>8\%$, occurring in the 15–25 km depth range, depending on the thermal gradient. Moreover, in the case of a cold lower crust, the consumption of plagioclase in favor of high-velocity minerals might represent another relevant seismic discontinuity. Different chemical compositions proposed for the Italian crust would be seismically indistinguishable, since they give overlapping seismic properties. Values of $V_s < 3.6$ km s$^{-1}$ would imply a strong contribution of sediments and/or partial melt. The $V_s$/density ratio shows a narrow variability, suggesting that densities at depth can be directly derived in first approximation from $V_s$.

1. Introduction

The Earth’s crust has been largely investigated through geophysical, geochemical, and petrological studies. Nonetheless, the origin, composition, and thermal structure of the crust remain unclear because of its heterogeneity and complex structure (Condie, 2013; Rudnick & Fountain, 1995; Rudnick & Gao, 2003; Taylor & McLennan, 1985; Windley, 1996). A better understanding of the crust is fundamental to infer its mechanical behavior, to define its role in plate tectonics, and to clarify the origin of magmas. In addition, better constraints on crustal features help to evaluate the contribution of the mantle in geodynamical processes as well as to isolate its signal in geophysical investigations (Ritsema et al., 2009; Tondi et al., 2012). Currently, there is an effort to merge different data and techniques in a multidisciplinary approach to reduce the ambiguities in crustal models. Examples are the joint inversion of receiver functions and surface waves (Bodin et al., 2012, 2016; Julia et al., 2000; Qashqai, Carlos Afonso, & Yang, 2016; Shen, Ritzwoller, & Schulte-Pelkum, 2013) or the simultaneous use of gravity and seismic data (Kaban et al., 2014; Tesauro et al., 2014a, 2014b; Tiberi et al., 2003; Vernant et al., 2002). To fully benefit from the combination of different methods, there is a need to reduce the uncertainty of geophysical models by setting robust and petrologically valid constraints. In order to accomplish this goal, it is essential to evaluate the contribution of each variable (temperature, pressure, composition, water content, and possible phase transitions) that affects seismic properties. One of the crustal features that we find not exhaustively explored in existing literature is the role of phase transitions. For example, the $\alpha-\beta$ quartz transformation (Shen, Bassett, & Chou, 1993) can show a clear signal in geophysical observations. In fact, $V_p/V_s$ anomalies have been recently linked to such transition (Kuo-Chen et al., 2012; Lowry & Pérez-Gussinyé, 2011; Mainprice & Casey, 1990; Mechie et al., 2004). However, the quartz structural change is not the only possible cause of variation in $V_p/V_s$ and its relevance compared to other sources of seismic anomalies is not yet fully understood.

A second important point to investigate is whether a mixture of different compositions (as those comprised below the wavelength of any seismic method) has seismic velocities that are equivalent to that of averaged and approximated mineralogical association.
With this work, we attempt to answer the main following questions:

1. Can we detect different chemical compositions within the crust using seismological studies?
2. What are the petrological constraints on the variability of $V_p$, $V_s$, density, and their relative ratios?
3. How do phase changes affect seismic properties in the crust?

In this study, we investigate the link between geophysical observables and crustal features, using thermodynamic modeling as a tool for the prediction of seismic properties in a wide range of pressure and temperature. Specifically, (i) we explore to which extent that the thermo-chemical characteristics of the crust can be revealed by seismic data, (ii) we determine the role of phase changes and melt, and (iii) we quantify their effects on different seismic observables (i.e., Rayleigh-wave dispersion curves and receiver functions). Finally, we detail the implications and pitfalls in the interpretation of seismological data for the crust. In this work we choose the Italian peninsula as a case study, due to the accessibility of several published estimates of its crustal composition, the presence of large temperature variations and locally high thermal gradients, and abundant and reliable seismological observations covering this area.

In the following introductory sections, before presenting and discussing our results, we provide an overview of the role of geophysics in the characterization of the crust, discuss possible constraints on crustal composition, and present the state of the art on the relationships between seismic observables and material properties.

1.1. Geophysical Studies of the Crust

Seismic studies and gravimetry have been largely used in the past decades to characterize the crust. Several crustal models have been proposed in terms of seismic velocities and density such as LITHO1.0 (Pasyanos et al., 2014), CRUST 1.0 (Laske et al., 2013), CRUST 2.0 (Bassin, Laske, & Masters, 2000), and GEMMA (Reguzzoni & Sampietro, 2015). In areas with dense data coverage, models with higher resolution have been provided such as the EPcrust model (Molinari & Morelli, 2011) and NACr14 (Tesauro et al., 2014a) for the European and North American continent, respectively.

The distribution of compressional velocity ($V_p$) at depth is obtained from the analysis of $P$ wave arrivals generated by earthquakes worldwide (teleseismic tomography) and/or from local events within the studied area. The obtained tomography images generally show good horizontal resolution on the order of tens of kilometers. For the Italian peninsula, regional, high-resolution tomographic studies have been carried out (Di Stefano et al., 1999, 2009; Gualtieri, Serretti, & Morelli, 2014). In addition, reflection seismic surveys (e.g., CROP project (Finetti, 2005)) have provided a relevant insight on the crustal structure of this region.

Shear-wave velocities ($V_s$) at crustal depth are mainly obtained through the analysis of surface waves, either generated from earthquakes or retrieved from ambient-noise interferometry (passive method). The vertical resolution of the obtained $V_s$ models is generally lower if compared to a $V_p$ tomography. However, the coverage is higher and more homogeneous, especially when using passive approach. Examples of recent crustal models from surface wave analysis are Molinari, Verbeke, et al. (2015) and Shen and Ritzwoller (2016), for the Italian region and North America, respectively.

Another geophysical technique employed for crustal studies is based on the analysis of receiver functions (RFs). This method was introduced in the late seventies (Vinnik, 1977) and largely developed only in the last decade. It is based on the analysis of converted $P$ and $S$ phases at seismic discontinuities beneath seismic stations (Zhu & Kanamori, 2000). The RF method is particularly suitable for detecting sharp layer boundaries, such as the Moho. Examples of application of this method for the Italian peninsula have been shown by Piana Agostinetti and Amato (2015) and Shen and Ritzwoller (2016), for the Italian region and North America, respectively.

As any geophysical method, the aforementioned techniques require an inversion of data to infer a velocity model of the subsurface. Factors such as noise in the data, the high number of parameters in the inversion problem, and uneven illumination of the subsurface require some regularization choices (e.g., smoothing) to help the convergence toward a final solution during the inversion procedure (Pasyanos & Walter, 2002; Vasco, Johnson, & Marques, 2003). As a consequence, the retrieved models might miss sharp discontinuities, even if present. Lastly, the solution to the inversion problem is often nonunique, as several models might explain the observed data equally well.
1.2. Composition of the Crust and Its Determination

Exhumed portions of the crust and xenolith catalogs have been extensively used to infer crustal composition in terms of main oxides and mineralogical associations (McLennan, Taylor, & Heming, 2005; Rudnick, 1992; Rudnick & Gao, 2003). It is widely accepted that the average composition of the crust is andesitic (Rudnick & Gao, 2003, 2014). However, both seismological and geological evidence (e.g., exhumed portion of the crust and xenoliths) show a compositional layering ($\text{SiO}_2$ content decreasing with depth) suggesting the compositionally distinct upper, middle, and lower crusts (Rudnick & Fountain, 1995; Taylor & McLennan, 1985). Considerable uncertainty exists especially regarding the lower crust. As a matter of fact, most of the information about its properties relies on xenolith samples whose depth of origin and representativeness of the lower crust are poorly constrained (Hacker, Kelemen, & Behn, 2015). With respect to the upper and especially middle crust, their thicknesses or even existence are often questioned.

Besides a globally inferred composition of the Earth’s crust, average chemical compositions have been also proposed for certain local domains. For this study, we use a range of compositions inferred for the Italian province, but we anticipate that our results might be extended to other areas. A comprehensive summary of the complex geological and geodynamic setting of the Italian region is beyond the scope of this work. Abundant literature is available in this regard and here we only mention some key points of interest in the context of this work. The current geological setting of the Italian region is determined by the Alpine and Apennine orogenesis started in the Cretaceous due to the convergence of the African and European continents (Carminati, Lustrino, & Doglioni, 2012; Doglioni et al., 1999; Mantovani et al., 2002). The position of the Italian peninsula results from the counterclockwise rotation of the Apenninic front (15 Ma to present) that led to the opening of the Tyrrhenian Sea basin (Carminati et al., 1998, 2010, 2012; Doglioni et al., 1999; Doglioni, Mongelli, & Pialli, 1998; Faccenna et al., 2001). Diffuse magmatism occurred in the Quaternary and is continuing at the present time (Carminati et al., 2010; Peccerillo, 2005). The recent tectonic evolution resulted in the high thermal gradients in the western Apennines ($\geq 150 \text{ mW/m}^2$), opposite to the lower values ($\sim 30–40 \text{ mW/m}^2$) found in the foreland areas of the Po Plain, Adriatic Coast, and the Ionian Sea (Della Vedova et al., 2001). Gravity and seismic data suggest that the crust is mainly continental, with a Moho at 30 km depth on average. The Alpine belt shows a higher crustal thickness ($45–50 \text{ km}$), while the Ionian and Tyrrhenian Sea are underlain by a (oceanic) crust around 10 km thick (Scrocca, Doglioni, & Innocenti, 2003, and references therein). Sassi (2003) provides several compositional averages based on extensive sampling of exhumed portion of shallow to deep crust, as in the area of Ivrea Verbano (Fountain, 1976). We will thus consider those averages to infer the correspondent seismic properties using thermodynamic modeling.

1.3. Merging Composition and Geophysical Observables

Finding a correlation among chemical composition, petrology, and seismic velocities has been a matter of research for decades. Several laboratory experiments explored the change in $V_p$, $V_s$, and density for several rock types (taken as representative of different portions of the crust) as a function of pressure (P) and temperature (T) (Birch, 1961; Christensen & Mooney, 1995; Rudnick & Fountain, 1995). Empirical relationships have been then derived to associate these variables to $V_p$, $V_s$, and density (Brocher, 2005; Ludwig, Nafe, & Drake, 1970). However, the simultaneous effects of pressure and temperature are only mildly considered in these studies, albeit P and T show an important role in controlling seismic velocities at depth. In addition, the empirical observations only span a limited temperature and pressure range, while in the crust these can be as high as 2–2.5 GPa and 1500 K, respectively. Therefore, such experimental relationships might not be reliable if applied to the entire crust (Guerrì, Cammarano, & Connolly, 2015). Finally, the use of the aforementioned empirical relationship neglects the effects of water and/or melt.

Some studies (i.e., Behn & Kelemen, 2003; Tassara, 2006) have proposed empirical formulas to derive major oxides content (e.g., $\text{SiO}_2$, MgO, and CaO) from seismic velocities, or vice versa. However, as already shown in the early studies by Birch (1961) and Christensen and Mooney (1995), rocks with very different composition and mineralogy show overlapping seismic properties. Thus, if such empirical fits are used, seismic velocities translate in a broad range of $\text{SiO}_2$ (e.g., if $V_p = 6.4 \text{ km/s}$, silica content ranges between 53 and 73 wt % at 20 km; see Behn & Kelemen, 2003). Therefore, the use of complementary information (such those on $V_S$ and density) and petrological constraints is fundamental to reduce ambiguities (Afonso et al., 2013). It is worth noting that empirical relations neglect possible phase transformations that might...
occur at crustal depths (e.g., quartz transition). Also, the role of melt, not negligible in zones with high thermal gradients, is not taken into account. Lastly, once a chemical composition is inferred from observed seismic velocities, its representativeness over the volume of investigation is not fully understood.

In this work, we use thermodynamic modeling to predict seismic properties at crustal conditions. Differently from laboratory experiments, this approach allows to evaluate the simultaneous effects of temperature, pressure, water content, composition, and possible phase change. Despite the theoretical nature of the employed method and the obtained results, important observations can be made to enhance our comprehension of the properties of crustal rocks at depth.

2. Data and Methods

We used thermodynamic modeling based on Gibbs Free Energy minimization (Connolly, 2009), a technique that predicts the stable mineral assemblage given a certain chemical composition and, self-consistently, calculates the seismic velocities and density of each mineral, for any point in the P-T space. The seismic properties of the (synthetic) bulk rock are then obtained by averaging schemes such as Voigt-Reuss-Hill (Hill, 1952).

We used the thermodynamic database from Holland and Powell (1998) with the shear and bulk moduli of minerals from Hacker and Abers (2004). The database includes the experimental results from Ohno, Harada, and Yoshitomi (2006) that accounts for the anomalous elastic behavior of quartz at the \(\alpha-\beta\) transition, useful for our specific intent to model crustal, quartz-bearing rocks. Abers and Hacker (2016) already implemented the peculiar properties of quartz in a thermodynamic framework, but their approach is not self-consistent since the equilibrium of mineral species is not assured for the ranges of P and T considered in their work. It must be pointed out that our method is also not internally consistent since the bulk and shear moduli are experimentally determined and not calculated as derivatives of the Gibbs free energy. While losing consistency, such approach is more flexible and allows the incorporation of experimental information of elastic properties of minerals that are key to explore the relationships between different physical properties (e.g., seismic velocities and density) of crustal rocks.

**Figure 1.** Locations of the considered average chemical compositions of the continental crust proposed for the Italian Province (listed in Table 1). Data are from Sassi (2003).
To quantify the role of chemical composition in affecting seismic properties, we considered eight chemical averages proposed for the Italian province (Sassi, 2003). These compositions refer to different geological domains (Figure 1) where crustal rocks are sufficiently exposed to provide a meaningful mean composition for the upper, middle, and lower crusts. Locations include the Alpine Orogen, the Calabrian, and Sicilian Arc, with lithologies including granitoids, sedimentary rocks, and metamorphic rocks. All compositions include the most abundant seven oxides, representing >99% of the whole chemical composition (Table 1). For the sake of comparison, we also consider the mean global composition of the crust proposed by Rudnick and Gao (2003).

For each considered composition we use thermodynamic modeling to retrieve (i) the mineralogical association stable at any crustal P and T condition and (ii) the seismic properties and density of the bulk rock. The same procedure above was applied considering the addition of 0.25 wt % of H2O to allow the formation of melt at temperature above solidus. Using thermodynamic modeling, the migration of melt is not accounted for, as it is considered in equilibrium with the restitic fraction. This permits to evaluate the contribution of melt in changing the seismic properties of the bulk rock. We decided to not consider the case of higher water content.

Figure 2 shows $V_S$ as function of temperature at 4 kbar, for an anhydrous and two wet compositions (0.25 and 1.0 wt % H2O, respectively). At subsolidus conditions, a water content higher than 0.25 wt % does not result in appreciable changes in seismic velocities, albeit giving petrologically different rocks. When the temperature is above the solidus, melt forms and $V_S$ drastically decreases by the same amount for the two hydrous compositions. This experiment illustrates that melts exert a dominant influence on seismic velocities, more than water content itself. Therefore, we opted for a minimum end-member in water content, set to 0.25 wt % in our thermodynamic modeling. A more detailed analysis of water-driven (second-order) effects on seismic velocities in the crust can be found in Guerri et al. (2015).

The seismic properties obtained from our modeling are presented in boxplots, one for each rock composition (Figure 3). Each rectangular box contains 50% of the data, within the first (25%) and third (75%) quartiles of the cumulative distribution, in the temperature range of 400–1,000 K and for portions of the upper, middle, and lower crusts. Our synthetic seismic velocities are compared with those from two seismological models covering the area of interest. These are the EPcrust model (Molinari & Morelli, 2011) and the one from Molinari,

Table 1

| Location                      | Composition | SiO2 | Al2O3 | FeO  | MgO  | CaO  | Na2O | K2O  |
|-------------------------------|-------------|------|-------|------|------|------|------|------|
| Upper crust                   |             |      |       |      |      |      |      |      |
| Eastern Peloritani Mountains  | EPM         | 66.5 | 17.6  | 6.1  | 2.3  | 1.9  | 2.9  | 2.8  |
| Serre Calabre                 | SC          | 68   | 16.2  | 5.4  | 1.5  | 3.4  | 2.9  | 3.6  |
| Western Peloritani Mountains  | WPM         | 66.4 | 18.1  | 6.3  | 2.4  | 1.7  | 1.9  | 3.4  |
| Eastern Alps                  | EA          | 68.8 | 16.8  | 5.1  | 1.6  | 1.5  | 2.6  | 3.7  |
| Rudnick and Gao (2003)        | RG          | 66.6 | 15.4  | 5    | 2.5  | 3.6  | 3.3  | 2.8  |
| Middle crust                  |             |      |       |      |      |      |      |      |
| Central Eastern Alps          | CEA         | 65.9 | 18.8  | 7.3  | 2.1  | 1.2  | 1.8  | 3    |
| Peloritani Mountain           | PM          | 65.3 | 19.9  | 8.1  | 1.8  | 0.4  | 1.2  | 3.3  |
| Rudnick and Gao (2003)        | RG          | 63.5 | 15    | 6    | 3.6  | 5.3  | 3.4  | 2.3  |
| Lower crust                   |             |      |       |      |      |      |      |      |
| Ivrea Verbano Zone            | IVZ         | 54.9 | 18.2  | 9.8  | 6.2  | 7.6  | 2.1  | 1.5  |
| Serre Calabre                 | SC          | 61.8 | 18.8  | 8.4  | 3.4  | 3.6  | 2.1  | 2    |
| Rudnick and Gao (2003)        | RG          | 53.4 | 16.9  | 8.6  | 7.2  | 9.6  | 2.7  | 0.6  |

Note. Arbitrary toponyms are given for each composition.
Verbeke, et al. (2015), MB from now on. The first is derived from the combination (i.e., weighted average; see reference for more details) of previous models covering the European continent. It is relevant to note that the VS and density of EPcrust are calculated through the empirical formulas of Brocher (2005) from the VP. The latter is a shear-wave velocity model derived from ambient-noise tomography from surface waves. The model is parameterized in upper and lower crusts and provides also VP (obtained from inversion) and density (fixed at 2.75 and 2.9 g/cm³ for the upper and lower crusts, respectively).

We also modeled the VP/VS ratio and acoustic impedances to highlight the role of phase transitions and/or compositional changes as possible seismic discontinuities. Finally, we constructed a whole synthetic crust parameterized in upper, middle, and lower crusts and computed the synthetic receiver functions (RFs) and Rayleigh wave dispersion curves along three geothermal gradients, in order to directly quantify the effects of the considered variables on seismic observables.

Figure 3. Boxplots showing the variation of VS, VP/VS, and the VS/density at temperature between 400 and 1,000 K for portions of the upper, middle, and lower crusts. Compositions labeled with “025” (identified with a blue-filled bar) contain H₂O at 0.25 wt %. The box includes 50% of the data within the first (25%) and third (75%) quartiles of the cumulative distribution. The black whiskers contain the majority of the data (~99%), and the red dots are the outliers of the distribution. The median is represented by a red line.
3. Results

3.1. Shear Velocity ($V_S$)

$V_S$ at crustal depths (upper, middle, and lower crusts) varies between 3.6 and 4.5 km s$^{-1}$ when compositions are anhydrous (Figure 3, left column). A strong variation with temperature, evidenced by larger "boxes" in Figure 3, is observed, especially in the upper crust. At relatively shallow depths, adding water causes the formation of melt at high temperature with the consequent reduction of velocities (Figure 3, top left). In the middle and lower crusts, the influence of water is remarkably less important, leading to overlapping $V_S$ ranges.

The MB model shows a wider distribution of $V_S$ in the upper crust. This is probably caused by the presence of sediments in the area covered by model, while we consider only a crystalline crust. The variability of $V_S$ becomes smaller at increasing depth and $V_S$ are lower than those determined from thermodynamic modeling. For the lower crust, the $V_S$ range from the MB model is close to those predicted for a hydrated composition.

The EPcrust shear velocities are systematically lower compared to those from thermodynamic modeling. Note that EPcrust is almost entirely based on $V_P$, while the $V_S$ values are empirically derived from Brocher’s relationship (Brocher, 2005). This suggests that the empirical fit might not be able to capture the variability of $V_S$ within the crust.

3.2. Compressional Velocity ($V_P$)

Results for $V_P$ are not shown due to their similarity to those for $V_S$. Compressional wave velocity changes as a function of temperature exclusively for wet composition, and only in the upper crust. The effect of water becomes negligible in the middle and lower crusts (where melt conditions are not reached), and $V_P$ exhibits similar average values and distributions, regardless of the composition. For an anhydrous crust, $V_P$ is bounded between 6 and 7.7 km s$^{-1}$, in the 5–30 km depth interval: the lowest value is reached at shallow depth (<15 km) for high temperature (1,000 K), while the highest value corresponds to the base of the crust at a temperature <500 K. In the upper crust, $V_P$ values of EPcrust are similar to those modeled for wet compositions. In the middle crust, EPcrust has $V_P$ that are close to those we model for the lower crust. The MB model shows substantially higher $V_P$ than those derived from thermodynamic modeling, especially in the upper and middle crusts. This discrepancy is likely due to the poor capability of surface waves in retrieving $P$ wave velocities at depth, as discussed later (see section 4).

3.3. $V_P$/Density

The highest variability of $V_P$/density ratio is seen mostly in the upper crust and for hydrated compositions (Figure 3, right column). Here the ratio ranges from 1 to 1.5. In the middle and lower crusts, the $V_P$/density ratio varies within a small range, roughly between 1.29 and 1.39, regardless the variable temperature and composition. The $V_P$/density obtained from the EPcrust model has also a narrow distribution, bounded in the same range we find from thermodynamic modeling. A significant discrepancy exists between the $V_P$/density estimated by MB and those we modeled. This is likely due to the assumption of fixed densities in the upper and lower crusts.

3.4. $V_P$/$V_S$

Figure 3 (middle column) is about the $V_P$/$V_S$ ratio. The lowest values are reached in the upper crust, comprised between 1.6 and 1.7. An increasing variability and higher values (up to 1.8) are observed deeper. For wet compositions, the formation of melt above the solidus ($T > 800$ K) yields values of about 2. However, at larger depths, both the effects of temperature and water become negligible and the medians of $V_P$/$V_S$ ratio stabilize between 1.65 and 1.75. EPcrust shows a narrow range of $V_P$/$V_S$, and its medians mostly overlap with those obtained from thermodynamic modeling. This is consistent with the fact the $V_S$ of EPcrust has been empirically derived from $V_P$. MB shows particularly high $V_P$/$V_S$. We explain this with the inability of data used to derive this model to provide plausible $V_P$ at depth.

We highlight the effect of quartz transition on the $V_P$/$V_S$ ratio in Figure 4. We consider here an anhydrous, simplified crust with the composition for the upper, middle, and lower crusts as in Rudnick and Gao (2003). The crust is 35 km thick, and it has the compositional boundaries between upper-middle and middle-lower crust at 15 and 25 km, respectively. We show the variation of $V_P$/$V_S$ along three linear geothermal gradients of 10, 30, and 40 K/km. A sharp decrease followed by an increase of $V_P$/$V_S$ is observed around 15 km depth for the highest thermal gradient (i.e., 40 K/km). The same feature occurs at 23 km depth for an average thermal gradient.
Figure 4. Variation of the $V_p/V_S$ ratio as a function of depth and thermal gradient. The compositions of the upper, middle, and lower crusts are from Rudnick and Gao (2003). For an average and high gradient, the sharp jump at 15 and 23 km is due to the transformation of $\alpha$-quartz in $\beta$-quartz occurring at $T = 900$–$1,000$ K. The effect of quartz transformation masks the one induced by the compositional change at boundaries.

Figure 5. $V_S$/density ratio as a function of temperature for two anhydrous compositions, Ivrea-Verbano Zone (IVZ) and Serre Calabre (SR), and for their 1:1 mixture (black). The dotted line represents the arithmetic mean between the $V_S$/density ratio of two compositional end-members.

(30 K/km). An inspection on the mineral association that is stable at these pressures and temperatures confirms that the change in $V_p/V_S$ is due to $\alpha$-$\beta$ quartz transformation. As shown by experiments in Ohno (1995), this phase transformation first induces a decrease in compressibility, resulting in a decrease of $V_p/V_S$ then is characterized by a rapid increase in $V_p/V_S$ (here up to 1.8) when the transformation is completed and quartz structure is stable in the stiffer and denser $\beta$ form. We observe that the jump in $V_p/V_S$ due to the $\alpha$-$\beta$ quartz transition is higher than the jump caused by the varying composition between layer boundaries, which is visible in Figure 4 for the lowest thermal gradient (10 K/km).

3.5. Seismic Properties of a Mixed Chemical Composition

Seismic tomography has a notoriously limited resolution, implying that observed seismic velocities are an average over volumes that include different crustal compositions and lithologies. Therefore, it is important to test whether an average composition in chemical equilibrium (that could be derived from a seismic model) would exhibit similar seismic properties and density of a mechanical mixture of different compositions. To address this point, we consider the compositions of Ivrea-Verbano Zone and Serre Calabre (here IVZ and SR, respectively) as end-members for the lower crust. We chose them as they show the highest relative difference in SiO$_2$, CaO, and MgO contents (see Table 1). In our test, we consider the $V_S$/density ratio, as this is the parameter that is possibly more sensitive to composition and less to pressure and temperature (see section 3.3). We computed the $V_S$/density ratio of a 1:1 compositional mixture of the chosen end-members, as a function of temperature (Figure 5, black line). We compare this with the behavior of a mechanical mixture, represented by the average $V_S$/density between the end-members (dashed line in Figure 5). In both cases, the $V_S$/density ratio change nonlinearly with temperature and, more importantly, are completely overlapping. This simple test shows that an average chemical composition has seismic properties that are indeed approximately equal to the average seismic features of the end-members.

3.6. Acoustic Impedance

In order to show the presence of possible seismic discontinuities, we plot the acoustic impedance, defined as acoustic impedance (AI) = $V_p \times$ density, in a depth-temperature domain (Figure 6). We considered a 35 km thick crust with the upper-middle and middle-lower crust transitions at 15 and 25 km, respectively, and using the compositions given by Rudnick and Gao (2003). The modeled layered crust enables us to compare the effects of compositional changes versus phase transitions as possible sources of seismic discontinuities.

An AI jump is clearly visible in the upper and middle crusts, at a temperature between 850 and 950 K depending on depth. This is due to the quartz transition in the upper and middle crusts, already mentioned for causing an increase in $V_p/V_S$ ratio (see section 3.4). In Figure 6, the dashed black line indicates the transition temperature that has a gradient of 0.0256 K/bar as defined by Shen et al. (1993). The higher quartz content in the upper crust (>20 wt %) produces here a more pronounced jump in AI, compared to that of the middle and lower crusts where quartz is less abundant. Interestingly, Figure 6 shows that compositional changes at the layer boundaries produce a relatively mild jump in AI at the upper-middle crust boundary.

In conditions of high pressure and low temperature at midcrustal depth, a sharp increase in AI is observed. Inspecting the mineral phases that are stable under these conditions (reported in Table 2), we note that the AI
Figure 6. Acoustic impedance (VP × density) as a function of temperature and depth in a three-layers, 35 km thick crust with compositions from Rudnick and Gao (2003). The black dotted curve indicates the temperature α-β quartz transformation temperature from Shen et al. (1993). This phase transition produces a jump in AI in the upper crust (due to its higher content in quartz), less pronounced in the middle and lower crusts. Another AI increase occurs at 5.7 kbar driven by the increasing pressure in isothermal condition at mid-crustal depth. Bold: P-T condition used for thermodynamic modeling. Italic: stable mineral species compositions from observed chemical composition from observed chemical composition from observed chemical composition from observed chemical composition from observed chemical composition from observed chemical composition from observed chemical composition. The reason may be due to the different compositions and thermodynamic data-water. Our investigation aims to clarify the relative weight of these variables in controlling seismic velocities and density.

We believe that this simplification might hamper the application of such formulas in certain crustal domains. Behn and Kelemen (2006) also used a thermodynamic approach, now implementing the role of melt and water. Our findings are not totally consistent with this study, in terms of modeled seismic velocities and mineralogical assemblages. The reason may be due to the different compositions and thermodynamic database used for calculations. For example, in our database, we account for the anomalous behavior of quartz that may show an important role in controlling seismic velocities within the crust, as will be discussed later.

We show that the seismic properties of the local compositions proposed for the Italian crust closely overlap to those of Rudnick and Gao (2003). This result suggests that an average global composition can be a reasonable approximation, also at local scale. Indeed, the error made by assuming a global composition is lower than the uncertainty arising from variations in temperature and melt, usually unknown at depth and poorly constrained by seismic methods. An additional uncertainty is due to the limited resolution of any seismic tomography. Any compositional change within the crust is likely smaller than the wavelength of propagating P and S wave. We showed that it would be impossible to distinguish between a 1:1 mechanical mixture of two rock types and their compositional average. Thus, when the chemical composition is assumed to be an average of two end-members, its seismic properties are also the average of the end-members. Observed seismic wave velocities at depth thus represent an average value over a certain volume and can be used to infer the average chemical composition over that volume. Lithological and compositional heterogeneities considered in this study might be beyond the resolution of any geophysical method. Temperature and/or phase transitions might play the dominant effect. The unawareness of the limits of geophysical models can be the principle reason for several misunderstandings between different communities in geosciences.

4. Discussion

4.1. Constraints on VP, VS, and Density

Based on thermodynamic modeling, we explored the variability of VP, VS, and density as a function of temperature, pressure, composition, and water content. Our investigation aims to clarify the relative weight of these variables in controlling seismic velocities and density.

We found that the possibility of discriminating between different compositions within the same crustal layer is prevented by the overlapping values of VP and VS. Our results confirm previous works in literature (see section 1). For example, Behn and Kelemen (2003) drew the same conclusion using an analogous thermodynamic approach. Despite the conclusion that different rocks have similar seismic properties, they proposed experimental fits to obtain chemical composition from observed VP. This leads to wide ranges of oxide content that can fit the same value of seismic velocity equally well. A problem with their approach is the assumption of no water and melt.

Table 2

Table 2: Stable Mineral Phases and Their Abundances (% vol) at 600 K and 4.2–5.7 kbar (Middle Crust), Obtained by Thermodynamic Modeling

| Pressure (kbar) | Temperature (K) | Acoustic impedance (AI) | Al jump (%) | Anhydrous | 0.25 w % H₂O |
|-----------------|-----------------|-------------------------|-------------|-----------|--------------|
| 4.2             | 600             | 18.5                    | 6.7         | 16.3      | 18.16        |
| 17              | 600             | 19.7                    | 19.4        | 19.5      | 21.59        |

| Pressure (kbar) | Temperature (K) | Acoustic impedance (AI) | Al jump (%) | Anhydrous | 0.25 w % H₂O |
|-----------------|-----------------|-------------------------|-------------|-----------|--------------|
| 4.2             | 600             | 18.5                    | 6.7         | 16.3      | 18.16        |
| 17              | 600             | 19.7                    | 19.4        | 19.5      | 21.59        |

Note: The used chemical composition is from Rudnick and Gao (2003). The jump in acoustic impedance (AI) is due to the consumption of plagioclase, driven by the increasing pressure in isothermal condition at mid-crustal depth. Bold: P-T condition used for thermodynamic modeling. Italic: stable minerals composing the bulk rock.
Among all factors, temperature is the most dominant in affecting $V_p$ and even more $V_s$, especially if water is present. We found that $V_s$ values as low as 3.6 km s$^{-1}$ can occur for a hydrated (crystalline) crust, above solidus temperature (900 K). Therefore, crustal domains with such low $V_s$ might be likely associated with the presence of partial melt. Low $V_p$ and $V_s$ are typical of sediments (which are common in the upper crust) and meta-sediments (at lower depth) that are neglected in this study. Their effects would give rise to distinctive anisotropies that would be visible both in surface-wave tomography and in receiver function studies. An example is reported in Hacker, Ritzwoller, and Xie (2014) where the low $V_s$ (<3.4 km s$^{-1}$) encountered in a certain portion of the Tibetan crust and the observed 6–7% radial anisotropy are interpreted as the combined effect of melt and horizontally oriented micas. For the case of the Italian peninsula, Ökeler et al. (2009) pointed out a strong anisotropy (>10%) in the Southern Apennines as result of a partially melted crust. The role of temperature must be taken into account especially in areas with high thermal gradients that can enhance the velocity reduction. It is the case of the Italian peninsula where anomalous thermal gradients are observed in areas of relevant magmatism (i.e., southern Tuscany, Tyrrhenian Sea, and Aeolian Islands). In Italy, the role of sediments can also be relevant. Examples are the basin area of the Po Plain where they reach a thickness of 15 km (Molinari, Argnani, et al., 2015) and the foreland of the Apulian Platform characterized by a 6–7 km thick carbonatic sequence that then dips under the southern Apennine fold-and-trust belt (Mariotti & Doglioni, 2000). Note that in our work we did not account for anelasticity, a phenomenon that could enhance the role of high temperatures in producing low seismic velocities (Karato, 1993; Watanabe, 1993).

We found that the $V_s$/density ratio takes a rather constant value around 1.34 km cm$^3$ s$^{-1}$ g$^{-1}$, despite the variable temperature, water content, and composition. In contrast with our result, Brocher (2005) found a nonlinear, fifth-order polynomial fit between $V_s$ and bulk density. The relation was derived from laboratory experiments based on a variety of rock types, but neglecting the simultaneous effect of pressure, temperature, water content, melt, and phase changes. On the contrary, in our thermodynamic approach, we account for these variables at once. Levandowski et al. (2015) and Levandowski, Boyd, and Ramirez-Guzmán (2016) proposed a correction to the Brocher's polynomial fit to account for temperature, assuming a constant thermal conductivity for the whole crust. In regions where conduction is not the only mechanism of heat transport, such as in zones characterized by large fluid circulation (a common case for the Italian province), this assumption might be too stringent. On the contrary, the substantial linear dependency between $V_s$ and density that we have derived accounts in first approximation for the possible role of temperature, water, and composition. It means that crustal densities might be first derived from a shear-wave velocity model. Of course, the use of gravity data would be necessary to validate and possibly improve the density model. We acknowledge that a possible reason for the narrow range of our modeled $V_s$/density ratio can be related to the thermodynamic database used in this study. In fact, for some minerals, the shear modulus is not available experimentally and their properties are approximated to those of known minerals with similar structure (Hacker & Abers, 2004). A comprehensive discussion of the uncertainty of thermodynamic properties of major minerals can be found in Hacker, Abers, and Peacock (2003). However, data do exist for most important crustal minerals, such as ortho-pyroxene, clino-pyroxene, and quartz (Anderson, Isaak, & Oda, 1992; Bina & Helffrich, 1992; Ohno et al., 2006). Better constraints on the mechanical behavior of minerals will hopefully give more reliable predictions on the characteristics of the crust.

The importance of using correct seismic constraints is demonstrated by the comparison of our thermodynamic data with two seismic models covering the Italian region. We observed that if seismic properties are empirically inferred, assumed, or poorly constrained, these are inconsistent with what thermodynamics suggests. A convincing example is given by the $V_p/V_s$ in the MB model. It ranges from 1.65 to 2.3, whereas both the EPCrust model and our modeled data show a much narrower range, centered around 1.7. MB is constructed from surface waves and thus is poorly sensitive to $V_p$. The absence of an adequate a priori constraint during the inversion stage produces unrealistic values of $V_p$ in the final model. In summary, we suggest that either (i) poorly constrained parameters should not be presented in the published model because its interpretation (from those unaware of this critical issue) can translate in wrong conclusions and (ii) petrologically valid constraints should be used to narrow the variability of such parameters. Thermodynamic modeling can give a valuable insight in this regard.
Finally, we stress that our method and results might be hardly applicable to the uppermost crust where the influence of pore and sediments might be dominant. In this work we simulated a crystalline, isotropic, pore-free mineral aggregate. Moreover, we did not take anisotropy into account, an important feature for seismic data if sediments or meta-sediments are present at depth. More complex thermodynamic modeling tools have been developed (e.g., HeFESTo from Stixrude & Lithgow-Bertelloni, 2011) to account for the full elastic tensor, but, as discussed earlier, there is a lack of experimental data in current databases even for isotropic properties.

4.2. Phase Changes as Seismic Discontinuities

Our results suggest that the α-β quartz transition has a considerable effect on the bulk properties of a crustal rock. We found that when the transition temperature (ranging from 850 to 950 K, depending on pressure) is approached, the $V_p/V_S$ ratio first decreases (<5%) and then increases up to a value of 1.8 or more. The depth of the quartz transformation is governed by the thermal gradient. Figure 7a clarifies the role of temperature gradient on $V_p/V_S$ when the transition of quartz occurs. A gradient between 28 to 40 K/km results in a quartz transition in the middle crust (15–25 km depth). Importantly, we show that the increase in $V_p/V_S$ due to this transition is higher than that driven by the compositional layering of the crust. If the thermal gradient is lower than 28 K/km, the quartz transition would occur in the lower crust. Its mild effect (mild because of the low quartz content) is masked by an increase in $V_p/V_S$ due to the compositional change at the middle-lower crust boundary. Mechlie et al. (2004) interpreted the high $V_p/V_S$ anomalies observed in Tibetan crust as evidence of the α-β quartz transition at around 20 km depth. Their interpretation assumes that the involved crustal rocks have a quartz content that is high enough (>30% vol) to yield a significant $V_p/V_S$ anomaly, as shown in Le Maitre (1976). In contrast, our thermodynamic modeling shows that a significant change in $V_p/V_S$ due to the quartz transition already occurs with less quartz content (<20% vol).

Figure 7. Relative change of $V_p/V_S$ in % from a value of 1.7 (median in the P-T space), as a function of depth and temperature gradient. Crust is 35 km thick with composition from Rudnick and Gao (2003). (a) Case of an anhydrous crust where the transformation of quartz is the major cause of the change of $V_p/V_S$. (b) Case of a wet crust where the formation of melt significantly increases $V_p/V_S$ above the solidus temperature, masking the α-β quartz transition.
Even if seismically relevant, the quartz transition is probably difficult to detect. Being not sharp (it occurs over a depth range of 3–5 km; see Figure 4), seismic methods with low vertical resolution (i.e., surface wave tomography) might not be able to resolve it. However, we think that the use of receiver functions would be beneficial for the detection of the α-β transition. A promising outlook is the use of this phase change as possible geo-thermometer, as first proposed by Mechie et al. (2004). The detection of this transition can also have major implications to determine crustal rheology at depth. In fact, close to the transition temperature, the Young’s modulus of quartz decreases by ~30% (Peng & Redfern, 2013). Therefore, if stress is applied, a quartz-bearing rock might undergo a relevant mechanical weakening near the transition temperature, favoring strain accumulation. An additional parameter that is affected at quartz transition is thermal conductivity. Gibert and Mainprice (2009) reported a minimum value of thermal conductivity of quartz at the α-β transition. If confirmed, this peculiarity would affect the geothermal gradient at the depth of the phase transition. Moreover, the latent heat absorbed for the transformation could decrease the thermal gradient even more, thickening the depth interval where the transformation occurs.

The increase in $V_p/V_S$ within the crust cannot be univocally interpreted as the α-β quartz transition. Temperature above solidus in a wet crust induces the formation of partial melt, causing a strong decrease in $V_S$ and thus an increase in $V_p/V_S$ ratio. Figure 7b shows the relative change in $V_p/V_S$ as a function of depth and temperature gradient in a wet crust. The raise in $V_p/V_S$ is caused by the presence of melt (~1% vol in our thermodynamic calculation) at depths and temperature that are close to those of the α-β transition. Hence, only considering the $V_p/V_S$ ratio can lead to a wrong interpretation. Both $V_p$ and $V_S$ data sets must be thus taken into account when interpreting variations in $V_p/V_S$. Note that the calculated seismic properties are reliable also at solidus and subsolidus conditions. Our thermodynamic computations make use of the comprehensive and extensively used database from Ghiorso et al. (2002) for phase relations between mineral aggregate and silicate melts. In contrast, we point out that our modeled $V_p/V_S$ are not reliable for temperatures that are too high above the solidus. This condition favors the production of large quantity of melt (>1–2% vol), causing excessively low $V_p/V_S$ in the bulk rock, as those seen in Figure 7 at $T > 900^\circ$C. The assumption made in our thermodynamic modeling that melt is in equilibrium with the mineral aggregate is not realistic in this case. Large amount of melt is unstable and tend to migrate from the restitic fraction.

Besides the quartz transition, we showed that the breakdown of plagioclase can also affect seismic velocities. Figures 6 and 7a show that it occurs at low temperatures (500–800 K) in the lower crust and mildly in the middle crust, causing an increase in acoustic impedance (>10%) and $V_p/V_S$ (7%). Here plagioclase is consumed in favor of dense, high-velocity minerals (e.g., clino-pyroxene). Interestingly, the associated sharp contrast in Al would exceed the effect of a chemical change at the middle-lower crust boundary. This implies that an observed sharp increase in seismic velocities is not necessarily associated with a change in chemical composition and/or the formation of garnet (that we find stable at higher pressures than those presented in our study). We conclude that the breakdown of plagioclase could play a significant role as seismic discontinuity. It could be even more relevant for anhydrous compositions, as suggested in Guerri et al. (2015).

### 4.3. Effects on Seismic Observables

Can we detect different compositions within the crust? And how do phase changes affect its seismic properties? To address these questions, we compute synthetic Rayleigh-wave dispersion curves and receiver functions using the $V_p$, $V_S$, and density profiles obtained through thermodynamic modeling.

Surface waves are sensitive to the $V_S$ profile at depth. For forward computation, we use a code based on Hisada (1994), Lai (1998), and Lai and Rix (1999) that retrieves the Green’s function for a vertically layered heterogeneous medium. On the other hand, receiver functions are sensitive to seismic discontinuities underneath seismic stations. We compute RFs using a Thomson-Haskell propagator matrix for layered media. Figure 8b shows the dispersion curves along three different thermal gradients (10, 30, and 40 K/km), for a 35 km thick crust with composition from Rudnick and Gao (2003), as so far. The average and high thermal gradients produce almost overlapping dispersion curves, due to the similar $V_S$ structure at depth regardless the different thermal gradients considered. Indeed, the $V_S$ profiles in the two cases are almost identical (Figure 8c). On the contrary, a low gradient of 10 K/km is associated with values of Rayleigh phase velocities that are remarkably higher, especially in the 15–25 s range.
The key role of quartz transformation emerges when computing synthetic RFs. The average and high gradients give similar RF waveforms, in both amplitude and phase. More importantly, these waveforms are dominated by the quartz transformation that affects both the $V_P$ and $V_P/V_S$. If such similar RFs are observed, they would lead to almost identical velocity profile after inversion. The difference with the case of a cold gradient ($10 \, K/km$) is significant. The arrivals are earlier (e.g., up to 2 s for the $PpShs + PsPhs$ phase) with respect to the "warm" waveforms. This is due to the higher $V_P$ and $V_S$ along the depth profile (see Figure 8c). Moreover, amplitudes of phases in the "cold" RF are lower, due to the small jump in Al and $V_P/V_S$ occurring at the compositional transitions.

Far from being an exhaustive example, this exercise shows that temperature largely influences seismic velocities. Same chemical compositions exhibit diverse velocity profiles that are controlled by the temperature distribution at depth. Temperature defines the seismic properties of minerals, their stability, and control mineralogical transformation. Therefore, independent information on the local temperature gradient is fundamental for an improved and reliable interpretation of seismological data of the crust.

5. Conclusions

In spite of abundant data, the formation, evolution, structure, and composition of the crust are still unclear and matter of debate. Geophysical methods provide biased information because of the strong nonuniqueness of the retrieved models, model assumptions, and nonlinearity of relations used to tie physical and seismic properties. In order to improve the interpretation of geophysical data in a multidisciplinary framework, we analyzed the effects of temperature, pressure, composition, and water content on the seismic properties of the crust in a thermodynamically consistent approach. Our major findings are summarized as follows:

1. Different dry compositions, typical of crystalline crust (note that we do not consider in this study a variety of sedimentary rocks that can characterize the top portion of the crust) can be seismically undistinguishable. The variation induced by a different composition is always lower than that caused by temperature and water content. The global chemical composition of the crust proposed by Rudnick and Gao (2003) provides similar seismic properties as those determined at a regional scale. Therefore, it can be used as a reasonable approximation for the chemical composition also for local studies.
2. In order to infer temperature and/or composition of the crust, it is necessary to use complementary geophysical data sets and thermodynamic constraints.

3. The $V_p$/density has an almost constant value around 1.34 for variable temperatures (400–1,000 K), pressure, dry composition, and water content. In absence of better constraints, this ratio could be used in joint-inversion of gravity and seismic data assuming a crystalline, pore-free rock.

4. The $\alpha$-$\beta$ quartz transition might represent an important seismic discontinuity in the middle crust (15–25 km). It is marked by an increase in $V_p$ and $V_P/V_S$, both larger than those generated by compositional changes at the upper-middle, middle-lower crust boundaries.

5. The increase in $V_p/V_S$ cannot be univocally referred to the quartz transition. In a wet crust, the formation of melt causes also a high $V_p/V_S$ due to the decrease in $V_S$. Therefore, a correct interpretation of seismological data must be based also on the joint interpretation of independent $V_p$ and $V_S$ data to discriminate between the two cases.

6. In the presence of a localized pressure gradient and temperature between 500 and 800 K, the plagioclase breakdown can produce an increase of acoustic impedance and $V_p/V_S$ in the lower crust. The change in seismic properties, also in this case, is higher than that caused by a chemical transition at the boundary between middle and lower crust.

The use of thermodynamic modeling in this work required some simplifications. First, seismic properties were modeled assuming the thermodynamic equilibrium of all phases for any pressure and temperature while, in reality, crustal rocks can be in a metastable condition. Second, our modeling assumes an isotropic and pore-free bulk rock. This simplification might not be valid in the shallowest crust where mineral might still preserve a preferential orientation and porosity can significantly decrease seismic velocities. In addition, temperature-induced anelasticity is not accounted for, and, as already mentioned, we did not thoroughly assess the effects of sedimentary rocks on seismic velocities that might not be negligible in the upper crust. The considerations of these effects would be a matter of further investigation, for a better understanding of crust in terms of its thermo-chemical characteristics.

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