Seismic Velocities of Rocks: Numerical Comparison of Calculated Data with Experiment

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Seismic properties of rocks are mainly a function of their mineral composition, crystallographic orientation of main rock-forming minerals, number and orientation of micropores and type of pore fluids. Two basic laboratory methods can be used for finding seismic properties of rock: experimental measurement on rock samples or computation based on single-crystal elastic constants. The advantage of the experimental method is that it is applicable to rocks with complex structure and composition and it directly shows the effects of pores under various confining pressures. However, as the direct experimental method can not be used for rocks whose primary composition has changed during their uplift and exhumation, it is convenient to substitute the experiment with the numerical method.

Here we present our methodical approach to comparative analysis of experimentally measured and calculated velocities of longitudinal elastic waves (P-waves) in rock samples. For experiment, an ultrasonic pulse-transmission method of Pros (1998) was used. The experimental apparatus is designed for spherical rock sample, which is placed in high-pressure vessel and rotated along two perpendicular axes. The measurements are carried out under confining pressure of 400 MPa to suppress the influence of micropores, and repeated in 132 directions to get the 3-D dataset.

For the calculation of P-wave velocities and numerical comparison with experimental results special computer program has been developed (written by R. Melichar). The calculation is based on finding the elastic stiffness tensor for an aggregate of all constituent mineral phases. For each mineral phase the crystallographic orientation distribution is measured using EBSD method. Then the elastic stiffness tensors of all phases is computed with use of single crystal elastic constants. Based on stiffness tensors, volume fractions and densities of mineral phases, the aggregate stiffness tensor can be calculated using selected elastic mixture rule.

As the experimental velocities are measured at 400 MPa of confining pressure, the calculated stiffness tensors of constituent mineral phases have to be pressure-corrected prior to further processing. After the unification of coordinate systems of the two datasets to be compared, discrete experimental data are interpolated and numerically compared with the calculated data in a dense grid. The spatial distribution of the deviations is visualised in stereodiagrams.

Basing on the results the suitability of the two methods and the applicability of various combinations of Voigt and Reuss elastic mixture rules can be discussed. These comparative analyses could also reveal the residual influence of microstructure or micropores s.l. on seismic properties, if it exists. Examples are given in the contribution.

References

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Can Ternary Feldspars be Used to Constrain the Metamorphic Conditions of High-Grade Meta-Igneous Rocks? Evidence from Orthopyroxene Gneisses, Bohemian Massif

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The presence of ternary feldspars in high-grade meta-igneous rocks, and the recognition of the thermometric significance of these feldspars, has led recent workers to postulate peak-metamorphic temperatures in excess of 1000 °C. However it needs to be established that such ternary feldspars are not in fact survivors from the original high-temperature crystallisation of the igneous protolith. After exsolution, the host and lamellae in the ternary feldspar grains may be stable throughout the following history as long as recrystallisation does not occur. Such a history can involve rehydration and metamorphism, even under H_2O-saturated conditions, with the compositions and proportions of the host and lamellae being modified to reflect the P-T conditions experienced. Some of the high-grade meta-igneous rocks from the Moldanubian of the Bohemian Massif that contain ternary feldspar preserve a substantial measure of their igneous heritage. Orthopyroxene-bearing gneisses include types that are barely affected by the metamorphism, whilst others require hydration of the igneous protolith prior to development of a metamorphic overprint. A key to establishing the igneous origin of the ternary feldspar grains is their preservation in garnets that are either themselves igneous, or of a relatively low temperature metamorphic origin

Decompression Plagioclase Rims around Metastable Kyanite Crystals in Moldanubian Granulites – a Clue to Equilibration Volumes in Water-Deficient Metamorphic Rocks

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Modern techniques of thermodynamic modeling and metamorphic condition estimates are critically dependent on knowledge of the effective bulk composition of the system in question. In the case of fluid-saturated rocks, the effective bulk composition is generally well approximated by the composition obtained by conventional whole-rock analysis. However, metamorphic reactions in water-deficient high-grade rocks, such as peridotites and granulites, are limited by chemical diffusion. In this case, the equilibration volume is small and the effective bulk composition must be estimated by other methods. Here we develop a method that is applied to constrain the equilibration volume and effective bulk composition that was relevant to the formation of a texture that evolved Moldanubian granulites as consequence of decompression.

The texture is manifest by plagioclase rims around metastable kyanite crystals. The domains over which this texture develops are often silica-undersaturated and contain mineral phases typical of low pressure/high temperature (LP/HT) metamorphism (spinel or corundum). These features also occur in felsic granulites collected in the NE corner of the Strážek Moldanubicum (Bohemian Massif). There, the high pressure (HP) mineral assemblage is composed of Grt-Ky-Bt-Plg-Kf-Qtz, but commonly kyanite is replaced by sillimanite suggesting the stabilization of the low pressure assemblage Grt-Sill-Bt-Plg-Kf-Qtz. In many low pressure (LP) samples, crystallization of plagioclase completely isolates metastable kyanite grains from the matrix.

In typical HP samples, kyanite is in direct contact with quartz and K-feldspar. Matrix is composed of randomly ordered small plagioclase (An_{18}), quartz and K-feldspar. Garnets are randomly distributed in the rock with no particular affinity with the kyanite domains. In several HP samples paragenetically early plagioclase coronas rim kyanite grains. In these samples it is possible to observe both reactants – quartz and kyanite – producing the plagioclase rim. In LP samples, kyanite grains are never in contact with quartz. The plagioclase is zoned, ranging from An_{22} at the kyanite side to An_{16} near the quartz side, in a radial thickness of 200–250 μm. This 'compositional gradient' is represented by an Al-rich/Si-poor and a Si-rich/Al-poor domain in the plagioclase that masks the primary contact between kyanite and quartz. The kyanite breakdown was not isochemical because the formation of plagioclase corona requires addition of Ca and Na to the Si and Al donated by reacting kyanite and quartz. Mg and Fe must also be supplied to the domain to form spinel and biotite.

Textural relationships indicate that plagioclase grains have partially replaced kyanite and that the formation of plagioclase aggregates between kyanite and quartz suggests reaction: $1Ky + 0.686\ Qtz + 0.965\ CaO + 3.435\ Na_2O = 1.462\ Plg$. For our analysis, Na and Ca are treated as mobile species because they must have been supplied from outside of the domain, and it is assumed that diffusion driven by chemical potential gradients was the main transport mechanism of these components. Although Na and Ca have high diffusion coeffiecients, the plagioclase coronas are thin (200 μm) and were probably limited by low diffusivities of Al and Si (Mongkoltip et al. 1983). These latter cations were thus relatively immobile and controlled the size of the plagioclase rim. Na and Ca must have been released from former plagioclase distributed in the matrix surrounding the kyanite crystals because plagioclase is the only phase containing the Na_2O component and its availability thus controls the development of the domain. This process was modelled thermodynamically (Connolly 1990) assuming local equilibrium. The resulting composition diagrams enables estimation of the equilibration volume around each kyanite grain, i.e., the matrix volume required to supply the nutrients Na and Ca.