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H*P*-H*T* mineral physics: implications for geosciences
Preface

Knowledge of the structure and properties of minerals plays the crucial role in understanding and interpreting geological and geophysical observations; without the input of such data it is not possible to derive a unique model for the structure and composition of the interior of the Earth at any level, whether in the crust or the lower mantle. Recent decades have seen great advances in the resolution and precision of geophysical and geological measurements, for example the development of high-resolution seismic tomography, that have driven the experimental community to provide more precise and accurate measurements of physical and thermodynamic properties of minerals and, in particular, their variation with temperature (T), *pressure* (P) *and composition. Such data are now used to interpret the results of seismic tomography in terms of temperature or compositional changes. The developments in geophysical observations have also demanded that experimental measurements of minerals be performed at ever greater extremes of well-characterised pressures and temperatures. These have, in part, been enabled by the advent of more intense and new types of radiation sources, the third-generation synchrotrons and new pulsed neutron sources, with which to probe minute samples of minerals in new ways at such extreme conditions. These experimental advances in achievable pressures and temperatures have tended to dominate the field of science that has become known as ''mineral physics'', yet at the same time there have been considerable developments at more modest temperatures and pressures particularly in the precision and accuracy of data and the pressure scale itself, to the point at which different methods can be used to provide complementary and consistent data. For example, phase equilibria can be determined directly by synthesis and quench experiments, and also indirectly from measurements of the thermodynamic properties of the phases together with the elastic properties, which themselves can be determined by many fundamentally different methods.*

Significant improvements in the precision and the accuracy of experimental measurements also now allow the effect of chemical substitution, sometimes at the per cent or ppm levels, on the physical properties of minerals to be investigated. Because of its impact on transport properties and rock dynamics, one of the most important topics in geosciences is how much water can be incorporated in nominally anhydrous minerals. But while the changes in thermodynamic properties can be measured, precise characterisation of the low water contents and speciation in complex mineral structures remains a challenge. Here lies another opportunity for the integration of new methods, not only the experimental spectroscopies enabled by modern developments in radiation sources and instrumentation, but also the power of computational simulations. They have the ability to directly span the microscopic to macroscopic length scales. Thus, while the direct interpretation of the vibrational spectra due to isolated OH groups within minerals of potentially low crystallinity is a challenge, ab initio *computer simulations of the structure can provide the interpretive tool that, in a unique way, can relate the vibrational spectra directly to the microscopic structure of the mineral. These developments over recent years thus allow mineral physics to provide data to support petrological and geological studies of the crust and upper mantle, in addition to the more traditional support of geophysics in studies of the very deep earth.*

This issue of the European Journal of Mineralogy *is formed of papers presented at the ''International Mineralogical School on H*P-H*T Mineral Physics: Implications for Geosciences'' organised by the Italian Mineralogical Group in the beautiful location of Bressanone (also known as Brixen) in the Dolomites of northern Italy. The purpose of the school was to review for students both the breadth and the details of the many methods of mineral physics, and to show how the results can be used by different Earth sciences communities, from petrologists to geophysicists, to model geological processes at all scales from the microscopic to that of the whole Earth. The school itself attracted about 60 participants from several countries, but many students were unable to attend. The publication of this issue is therefore intended to provide to a far wider audience the same review of mineral physics and its applications, and to demonstrate in particular that mineral physics retains a dynamic and essential role for understanding the whole Earth from crust to core, and is not restricted solely to experiments at extremes of pressure and temperature.*

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The issue begins with a review combined from the presentations of three of the invited lecturers at the Bressanone school. It covers both the theory and measurement of elasticity, the material property that is central to understanding the structure and properties of the Earth, and other planets, because it is the property that determines both density variation with pressure and seismic wave speeds of minerals. The review provides a comprehensive overview of the physical principles and the capabilities of the experimental techniques now available. The development of elasticity measurements reflects the development of mineral physics as a whole; in the last half-century not only have many new techniques been developed and been made routine, but the pressure and temperature ranges accessible and the precision and accuracy of the results have increased dramatically. The following paper by Jackson et al. *illustrates one such example, the use of nuclear resonant inelastic X-ray scattering to provide the sound velocities of (Mg,Fe)*SiO_3 *orthopyroxenes by directly probing the partial phonon density of states of a resonant isotope of iron within the crystal structure. The basis of mineral behaviour is, of course, the atomic structure of minerals. The following five papers illustrate how a variety of structural and crystal-chemical problems can now be investigated by using single-crystal X-ray diffraction under high-pressure and high-temperature conditions. The accuracy and precision of the data that can now be collected with modern instruments and software allows the study of the structural evolution of minerals with a great structural complexity and low symmetry such as feldspathoids (Gatta* et al.*), chlorite (Zanazzi* et al.*) and prehnite (Detrie* et al.*), and to evaluate the effect of chemical substitutions on the physical properties (Boffa Ballaran* et al.*). The paper by Camara* et al. *illustrates how the analysis of spontaneous strain arising from structural phase transitions can be used to characterise the transition.*

The first group of papers in this issue therefore illustrates that the measurement and characterisation of the structure and properties of single crystals of minerals is mature and well-understood. The second group of papers illustrates the challenges, and some of the successes, of measuring the kinetic and transport properties of aggregates and rocks so important for understanding the dynamics of the Earth's interior. The relatively new technique of complex impedance spectroscopy is used by Romano et al. *to determine the evolution of electrical conductivity in wadsleyite as a function of water content. Ferdortchouk* et al. *apply variable oxygen fugacity (*fO_2*), at different* P-T *conditions, to evaluate the effect of* fO_2 *on diamond preservation and to examine the development of secondary diamond morphology. Bonadiman* et al. *show how the water content of pyroxenes, determined with accurate FTIR data, may be related to the petrological environment. The last paper of this issue illustrates how data on mineral and rock properties can be employed in state-of-the-art petrological-thermomechanical 2D numerical computer modelling. Gerya* et al. *describe, with a mass of provocative images, different possible scenarios of the evolution of subducted ridges as a function of different physical parameters.*

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