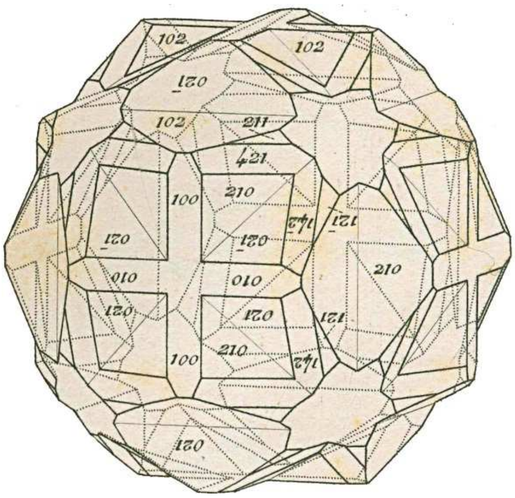

Impact of Crystallography on Modern Science

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Unraveling the Secrets of the Inner Earth by Means of a Computer: Mechanisms of Compressibility and Thermal Expansion of Crystals from a Theoretical Point of View

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The inner structure of the Earth and its dynamics are relatively well known, at least at the global scale and at the general level. The *shell* structure, consisting of (*i*) a crust; (*ii*) an upper and lower mantle divided by a transition zone; (*iii*) an external liquid, and an internal solid metallic core, is part of a widely accepted model derived from quite a large number of sources of information.

A crucial role in the construction of a realistic model of the Earth is played by *seismic tomography* which is used either (*i*) to provide direct data concerning the presence of discontinuities at several depths along the Earth radius, together with the elastic properties of layers crossed by the seismic waves along their journeys from the earthquakes' hypocenters to the seismic stations located all around the World, or (*ii*) as a test of consistency of the structural model proposed for our Planet: in fact, such a model must be able to provide the rheological properties of rocks from the Earth's surface to the core, which should agree with those derived from seismic tomography. Moreover, due to the complexity of the Earth's structure, the very interpretation of data from the seismic technique is not possible without an *a priori* knowledge of a reasonably accurate model of the inner Earth. From this point of view, both the Earth's model and the base knowledge required to correctly interpret data from seismic tomography are *self-consistently* refined in a cycle where results from one step serve as an input to the subsequent one, whose output is reintroduced as input to the first step, until self-consistency is reached to the desired level of accuracy and scale size.

A central key of such cycle is the knowledge of the elastic properties (*e.g.* compressibility), together with their temperature dependence, of materials supposed to be present at various depths. Indeed, the relevant properties of crystals can in many instances be experimentally determined, at high pressures, by X-ray diffraction techniques in diamond anvil cells (DAC). However, technical difficulties prevents the accurate measurements of the compressibility at simultaneous high pressure and temperature (HP/HT) conditions which are those typical of the Earth's mantle and core. In this case, HP/HT *first principles* simulations of structure and properties of crystals can provide an important support. In test cases, at room temperature, the difference between the calculated and the experimentally measured compressibility is very often within the error bar estimated for the best experimental data available. On the computational side, at variance with the experiment, such accuracy is expected to be preserved even at high temperature conditions, so that the computed thermo-elastic properties can confidently be used to refine the Earth's model and to correctly interpret the data from seismic tomography. As a *side product* of computations, the dynamics and the ultimate reasons of the thermal expansion of crystals, or their reactions to the applied stresses, or else their anomalous and critical behavior in proximity of phase transitions can be traced back to first principles, at the quantum-mechanical level.