Computational mineral physics: Past, present and future

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Mineral physics uses our understanding of the physical and chemical properties of minerals to interpret deep Earth geophysical structure and processes. In recent years, computational mineral physics has emerged as a complementary approach to experiment, as it can now be used accurately to determine the high pressure and temperature properties of minerals and hence provide insights into the nature of the deep Earth. A brief history of computational mineral physics will be presented, and the importance of the interplay between theory, experiment and computational simulation will be highlighted, as will the role played by Ron Cohen in the development and establishment of this field. Some of the current problems with our mineralogical interpretation of the deep Earth will be discussed, and the future opportunities that new instrumentation and computational facilities offer will be highlighted.

Crustal influences on U-Th disequilibrium at Ngauruhoe and Ruapehu volcanoes, New Zealand

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Ngauruhoe and Ruapehu are andesitic volcanoes located at the southern end of the Taupo Volcanic Zone in North Island, New Zealand. They are spatially separated by only 15 km yet each has an eruptive history and shows geochemical behaviour indicating separate and distinct magmatic systems. For each volcano U-Th isotopic data for young (< 3 ka) volcanic rocks show disequilibria that define an inclined array on the equiline diagram. Price *et al*. (2007)[1] have demonstrated that for Ruapehu the slope of the array has no time significance and is an artefact of mixing processes involving multiple fractionating andesitic magma batches and crustal assimilation. New U-series data for Ngauruhoe show very similar patterns to those observed at Ruapehu but, on the equiline diagram, Ngauruhoe data define an array with a slightly different slope and a distinctly different intercept on the equiline. The Ngauruhoe samples showing least disequilibrium are those with the highest $^{87}Sr/^{86}$ isotopic ratios and there is also a correlation between eruption age and Sr and Nd isotopic composition. In combination with major and trace element data, the isotopic systematics indicate that Ruapehu and Ngauruhoe andesitic magmas have evolved through a combination of closed and open system crystal fractionation and mixing but in each case the crustal assimilant is compositionally different.

[1] Price *et al.* (2007) *Chem. Geol.* **244,** 437-451.