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# Controls on trace element distribution in oxides and silicates

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Understanding and quantifying the partitioning of elements in low concentrations is important for petrology, as minor and trace elements are used as tracers of many geological processes. The lattice strain model of Blundy and Wood (1994) has consequently been found very useful, as it links mineral/melt partition coefficients to the elastic properties of the mineral and to the difference in ionic radius between the trace element and the cation it replaces. However, this model has limitations, particularly in terms of describing crystal strain, due to the form of the equation and from the choice of a hard-sphere model.

In a recent publication (Dubacq and Plunder, in press), we review the thermodynamics of trace element incorporation into crystal sites and equilibrium between mineral phases, and present classical atomistic modelling using transferable empirical potentials. Following incorporation of one (or more) mismatching element(s), crystal strain appears strongly related to the environment of the site of exchange, with anisotropic, vacancy-rich minerals deforming more than densely-packed minerals, due to anisotropic deformation, rotation and tilting of the surrounding polyhedra. In strained crystal sites, bond strain is smaller than the difference in cation radii, and varies between structures, with densely-packed minerals being less strained. Consequently, computed relaxation energies are smaller in less compressible minerals. This has implications for modelling the partitioning of trace elements, and highlights the limits of using continuum mechanics below crystal cell scale. Neither oxides nor silicates have isotropic elastic properties, and at nanoscale they do not deform like continuous material.

Predictions of partitioning between minerals, or between mineral and melt (or fluid) remain hampered by several factors, amongst which i) knowledge of the thermodynamics properties of the dissolved species (in melts and fluids), ii) the precision of estimated defect and strain energies and iii) the presence of solid solution in natural systems, even when limited to a few percent. The latter may have orders-of-magnitude effects on the calculated partition coefficients due to interactions between strain fields around minor cations.

Application and discussion of these concepts are presented for mineral/melt partitioning and for partitioning between minerals, using garnet/clinopyroxene equilibria. Advantage of the present approach is that it does not rely on fitting. Agreement with experimental data shows predictive accuracy within an order of magnitude, validating the theoretical approach and sufficient for application to some petrology problems. Improvements of the modelling for better application to minerals involve systematic work on the effect of solid solutions on the strain field around defects.

Dubacq B., Plunder A. (2018, in press) Controls on trace element distribution in oxides and silicates. *Journal of Petrology*

Blundy J. & Wood B. (1994) Prediction of crystal–melt partition coefficients from elastic moduli. *Nature* **372**, 452–454. doi: 10.1038/372452a0.