Goldschmidt 2000
September 3rd–8th, 2000
Oxford, UK.

Journal of Conference Abstracts
Volume 5(2), 138

Mineral Simulations at High Temperatures and/or High Pressures – Monte Carlo, Lattice Dynamics and Ab Initio Studies

Neil L. Allan (n.l.allan@bris.ac.uk)[1], **Jon D. Blundy**[2], **John A. Purton**[3] & **M. Yu Lavrentiev**[1]

[1] School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK
[2] Department of Earth Sciences, Wills Memorial Building, Queens Road, Bristol BS8 1RJ, UK
[3] Daresbury Laboratory, Warrington, Cheshire WA4 4AD, UK

Ab initio, Monte Carlo and lattice dynamics are increasingly able to provide valuable information concerning the behaviour of "perfect" and disordered minerals over a broad range of temperatures and/or pressures (e.g., Allan et al. 2000). This presentation focuses on two recent projects:

(a) Changes in the bulk modulus at the B1-B2 transition (Sims et al. 1999), using ab initio and pair-potential models. Results for bulk moduli and phonon frequencies will be compared with the data of Hofmeister (1997).

(b) New techniques for the simulation of solid solutions and disordered systems. Simulations have been largely restricted to end-member compounds, excluding many naturally occurring minerals. We have recently developed new methods for the calculation of free energy of solid solutions of ceramics and minerals at elevated temperatures and/or high pressures and hence phase diagrams (for our first studies see Allan et al. 2000). We concentrate on the two complementary strategies we have found most useful: (i) exchange Monte Carlo and hybrid Monte Carlo techniques (ii) full free energy minimisation via a combination of lattice statics and quasiharmonic lattice dynamics. Vibrational effects, ionic relaxation and configurational disorder are taken into account in both methods. (ii) is particularly useful for entropies of mixing, which automatically include both configurational and vibrational contributions therefore, no assumptions are made as to the ideality or regularity of the solution. We illustrate (i) and (ii) with a range of examples from oxide and silicate solid solutions, including perovskites and garnets, containing (a) Mn^{2+} and Mg^{2+} ions (b) Ca^{2+} and Mg^{2+}.

Allan NL, Barrera, GD, Purton JA, Sims CE & Taylor MB, *Phys. Chem., Chem. Phys.*, **2**, 1099-1111, (2000).

Sims CE, Allan NL & Barron THK, *Phys. Rev. B*, **60**, 2968-2971, (1999).

Hofmeister AM, *Phys. Rev. B*, **56**, 5835-5855, (1997).