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

Journal of Conference Abstracts
Volume 5(2), 922

Constraints on Core-Mantle Equilibrium: Metal-Oxide Partitioning of Ni, Co and Zn at High Pressure

David M. Sherman (dave.sherman@bris.ac.uk)

Dept. of Earth Sciences, University of Bristol, Bristol BS8 1RJ, UK

In stony-iron meteorites, siderophile elements partition into metallic iron over coexisting oxides and silicates. Based on the inferred concentrations of siderophile elements in the Earth's mantle, it has long been argued that the Earth's core and mantle are not in chemical equilibrium (Ringwood, 1972). However, a number of experimental investigations have suggested that element partitioning at high pressure may be different from that at 1 atmosphere. On the other hand, it is very difficult to measure element partitioning from runs performed in the diamond anvil cell. An independent prediction of element partitioning done from first-principles quantum mechanical calculations would be helpful. To this end, I have calculated the static enthalpy of the reactions $(M_{0.25},Fe_{0.75})$ + $(Fe_{0.25},Mg_{0.75})O$ = Fe + $(M_{0.25},Mg_{0.75})O$ for M = Co, Ni and Zn. Calculations were done using a plane-wave basis set with ultrasoft pseudopotentials and total energies were calculated using density functional theory in the generalized gradient approximation. Element partitioning is strongly affected by the pressures of the lower mantle (Figure. 1): The siderophile behavior of Ni decreases and becomes close to that of Co; Zn becomes much more lithophile at high pressure. Consequently, the high Ni contents of the mantle cannot be invoked as evidence for core-mantle disequilibrium. The increased lithophile behavior of Zn, however, helps support recent geochemical arguments about core-composition: Dreibus and Palme (1996) argue for a low-sulfur core based on the apparent Zn contents of the mantle, the absence of Zn partitioning into the core, and the relative volatility of Zn vs, S. The absence of pressure-induced siderophile behavior for Zn supports their assumptions.

Dreibus, G, and Palme H, *Geochim. Cosmochim. Acta*, **60**, 1125-1130, (1996).

Ringwood, AE, *Composition and Petrology of the Earth's Mantle, McGraw-Hill*, 618, (1975).

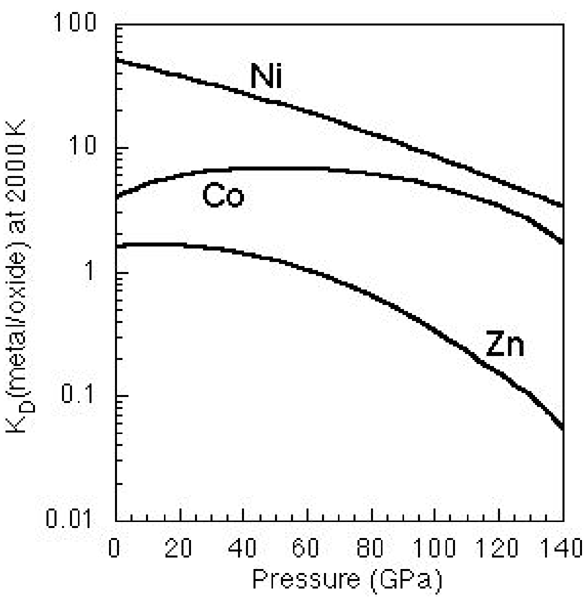

Figure 1: Predicted metal-oxide partition coefficients at 2000K