LIGHT ELEMENTS IN THE CORE AND DEGREE OF CHEMICAL EQUILIBRATION DURING CORE-MANTLE SEGREGATION: A WINDOW THROUGH FIRST-PRINCIPLES MOLECULAR DYNAMICS.

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Introduction: The degree of core-mantle equilibration degree (hereafter as Ke), defined as the fraction of the mass of the core in equilibrium with the mantle during the core-mantle segregation process in the early history of the Earth, greatly influences determination of the timing of the Earth accretion process [1]. If Ke is larger than 0.4, Hf-W chronology implies a fast accretion process in less than 30 Myr. Otherwise, Hf-W data can only be used to constrain the Ke instead of timing [1]. Here we use the two-phase first-principles molecular dynamics (FPMD) [2] to constrain the solubility of light elements in liquid iron in equilibration with silicate melt at relevant pressures and temperatures. The data, combined with various accretion scenarios of the Earth and light element content of the core, allow us to constrain Ke. Furthermore, the partition coefficients allow us to distinguish major and minor light elements in the core. In particular, the inferred carbon content of the core support Pb partitioning to the core [3].

Results: The two-phase FPMD simulations are performed for the system O-Mg-Fe-Si at temperatures from 2500 to 4200 K, pressures from 20 to 120 GPa, and two compositions simplified from the “O-bearing” and “Si-bearing” bulk Earth model compositions of McDonough [4] and expressed in wt% as follows.

	O	Mg	Fe	Si
Si-bearing	29.23	18.41	36.50	15.85
O-bearing	30.40	18.55	36.77	14.29

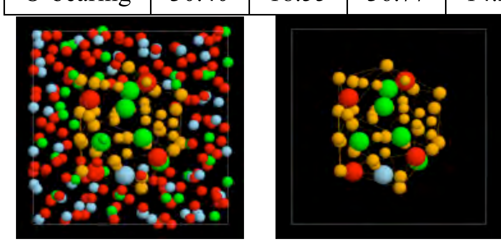

Fig. 1. A snapshot of FPMD at 4200 K and 120 GPa with O-bearing bulk composition. red=oxygen, sky blue=Mg, yellow=Fe, green=Si. Bigger O, Si and Mg are those included in the Fe-cluster. The right figure shows the “model Earth” while the left figure is “model core”.

After ~20,000 molecular dynamics steps, the atoms randomly distributed initially are segregated into two phases, one is liquid iron and the other is silicate melt. A snapshot of the final resulting configuration is shown in Fig. 1. Atom positions accumulated for ~ 40,000 steps are used to calculate the solubility of Si and O by computational geometry methods [2].

Solubility of Si and O in liquid iron. Fig. 2 shows the close agreement of solubility of Si in liquid iron predicted for systems having O-bearing and Si-bearing compositions with experimental results [5,6].

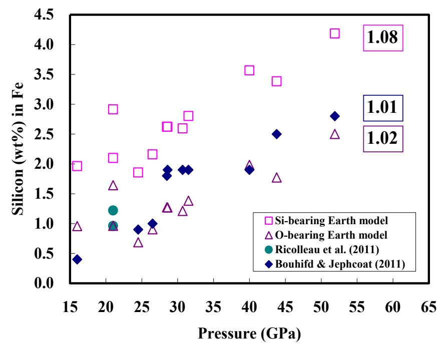

Fig. 2. The numbers in the rectangles are the total cation to oxygen mole ratios. The starting composition of Bouhifd and Jephcoat [6] is closer to that of the O-bearing model.

Construction of accretion models. Many different accretion routes can be constructed [7]. The starting point of the accretion routes is an embryo with 0.1 mass fraction of the Earh and a magma ocean depth of 20 GPa. The depth of the magma ocean at each accretional step (marked by the symbols in Fig. 3) is determined by the final magma ocean depth which is set as a variable (from 20 to 120 GPa).

Other variables considered include homogenous or heterogeneous accretion of the Earth, temperature along mantle solidus or liquidus, core-mantle equilibration degree, the accretion step when the non equilibrium between core and mantle starts. A computer program is made to run all the possible combinations of these parameters (~400,000 combinations in total) , and those that satisfy the light element content of the core are selected as plausible solutions. In running the program, we calculate two parameters for each accretion route. One is the effective magma ocean pressure (P_e):

$$P_e = \sum_i^N P_i / N \qquad \text{Eq. (1)}$$

where Pi is the magma ocean pressure for the ith accretion step, and N is the total accretion step. Another parameter is the effective core-mantle equilibration degree (K_e),

$$K_e = \sum_{i}^{N} Ke_i \times W_i \qquad \text{Eq. (2)}$$

where Ke_i and W_i are the core-mantle equilibration degree and the accreted mass fraction of the ith step. P_e and K_e reflect the accumulated and averaged magma ocean pressure and core-mantle equilibration degree.

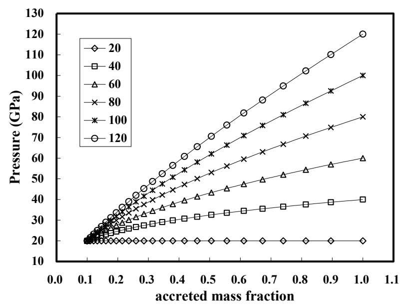

Fig. 3. Pressure at the base of a magma ocean along with the mass accreted at each accretion step (the lines mark the accretion routes).

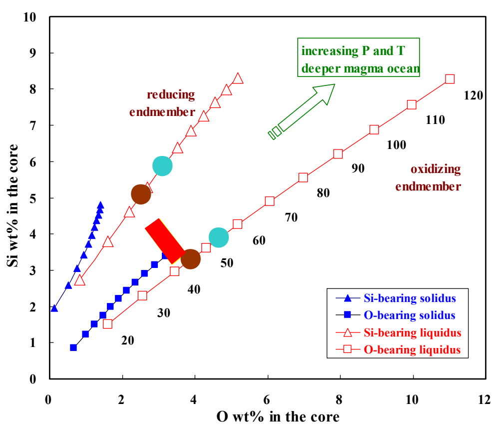

Fig. 4. Solubility of O and Si along mantle solidus and liquidus for systems having O- and Si-bearing bulk compositions. The numbers along the oxidizing endmember are the pressures (in GPa) on the liquidus. Symbols along other lines have similar order in pressure. The brown and aqua green circles give the O and Si content in the core with and without 2.0 wt% S in a single stage magma ocean process, respectively. The big red box covers the range of O and Si wt% from multi-stage Earth accretion models.

Valid parameter space. The successful parameter combinations give Si and O content of the core in a narrow range (the red box in Fig. 4). Most importantly, all the effective core mantle equilibration degrees are found to be larger than 0.57 (Fig. 5).

The Hf-W isotope system is used to infer the timing of core-mantle differentiation [8]. The high core-mantle equilibration degree found in the present study implies that the core-mantle differentiation has to occur early [1], within 30 millions years from the beginning of the solar system as originally stated [8].

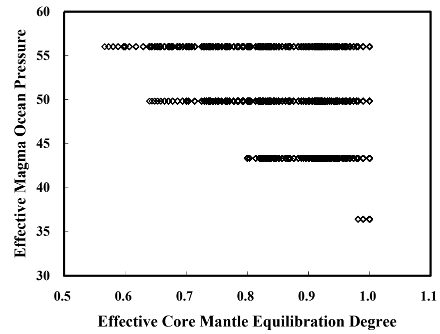

Fig. 5. Distribution of valid parameters of P_e and K_e that satisfy O and Si content of the core.

Carbon and other light-element contents of the Earth's core. Additional simulations (all at 3200 K and 40 GPa) were also made to calculate the partitioning coefficients of several other light elements. Combined with the bulk Earth compositions of these elements [4], they permit us to infer the light element contents of the core (Fig. 6). Si, O, and S are the major light elements in the core while C, P, Mg, H, and N are minor elements in the core. The impact of lower carbon content to the siderophile and chalcophile element distribution in the Earth's core and mantle will need to be critically evaluated.

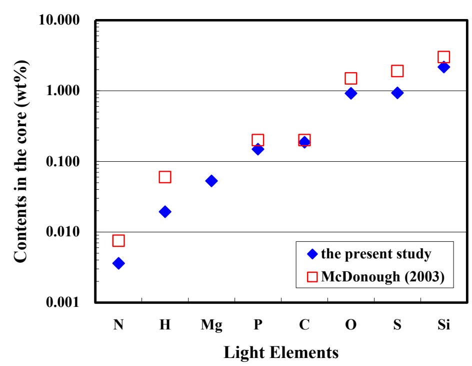

Fig. 6. Comparison of inferred light element contents of the core with ref. [4]. General agreement between the first-principles molecular dynamics calculations from this study with those of classical geochemical mass balance approach [4] are remarkable.

References: [1] Rudge J. F. et al. (2010) *Nature Geosci., 3,* 439. [2] Zhang Y. G. and Guo G. J. (2009) *GRL, 36,* L18305. [3] Wood B. J. and Halliday A. N. (2010) *Nature, 465*, 767. [4] McDonough W. F. (2003) *Treatise Geochem., 2,* 547. [5] Ricolleau A. et al. (2011) *EPSL, 310,* 409. [6] Bouhifd M. A. and Jephcoat A. P. (2011) *EPSL, 307,* 341. [7] Rubie D. C. et al. (2011) *EPSL, 301,* 31. [8] Yin Q. Z et al. (2002) *Nature,* 949.