Structure of grain boundaries in silicate materials (olivine and K-feldspar) applying focused ion beam (FIB) specimen preparation and TEM

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Our present knowledge on structure and behaviour of grain boundaries in silicates is still moderate compared to grain boundaries in metals and oxide materials. Various properties of silicates might be significantly influenced by the presence of grain boundaries and the grain boundary atomic structure. Structural grain boundary models derived from investigations on metals and oxides are frequently applied to silicates. Is such an assumption justified? There are similarities in the grain boundary structure. Melt films are observed along olivine grain- and olivine-pyroxene phase boundaries (Wirth, 1996). They are similar to amorphous films along interfaces in Si_3N_4 material (Kleebe *et al*., 1993).

However, there are also differences in the grain boundary structure. Based on the visibility of dislocation contrast in the TEM, the transition of low-angle to high-angle grain boundaries is suggested to be in the range of 10 – 15° of misorientation between the adjacent grains. Is this rule applicable to silicate grain boundaries? TEM grain boundary investigations on forsterite bicrystals synthesized by direct bonding question that transition range of 10 – 15°. In a recent paper by Heinemann *et al*. (2005) it was demonstrated that even at 21° misorientation of two adjacent forsterite grains, arrays of individual dislocations were observed. This observation suggests a different grain boundary structure from that of metals. In silicate grain boundaries charge compensation is a crucial requirement in contrast to grain boundaries in metals and therefore, a different grain boundary structure in silicates should be expected.

References

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The abundances of nominally chalcophile trace elements in the main minerals of upper mantle rocks

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Knowledge about the behaviour of the nominally chalcophile trace elements As, In, Sn, and Cd in the Earth's mantle is important to understand accretion, core formation, or the Earth evolution models. The abundances of these elements in the main minerals of upper mantle rocks are unknown. We present the required data, estimate inter-crystalline partition coefficients and Earth mantle abundances for these elements and demonstrate the lithophile nature of In, Sn and Cd in the upper mantle.

The trace element abundances in the minerals were measured in situ by LA-ICP-MS on polished thin sections of 20 spinel lherzolite and clinopyroxene-bearing harzburgite xenoliths hosted in alkali basalts from worldwide intra-plate volcanic fields. The xenoliths cover a large range of equilibration temperatures (from 850 to 1250°C) and are well-equilibrated with respect to major elements and lithophile and siderophile trace elements (e.g. REE, Sc, HFSE, Co, Ni). Most of the samples are free of visible sulfides except for the xenoliths from Kilbourne Hole carrying up to 0.1 % modal Fe-Ni-Cu-sulfides.

The main host phases for the elements In, Sn and Cd are clinopyroxene (13-58 ppb In; 48-527 ppb Sn; 37-149 ppb Cd) and if present, amphibole (49-58 ppb In; 248-649 ppb Sn; 53-89 ppb Cd). The contents in the sulfides are so low (sulfide/clinopyroxene ratio < 5) that the contribution of sulfides to the bulk rock abundances of these elements is negligible. In contrast, Arsenic is to a larger extent stored in sulfide (sulfide/clinopyroxene ratio > 100). All elements show systematic partitioning trends among the main minerals as function of temperature providing evidence that inter- and intracrystalline chemical equilibrium between the coexisting phases of the peridotites is achieved. The effect of increasing temperature is to redistribute the elements from clinopyroxene into orthopyroxene and even olivine. A very good coherence in the Dcpx/opx of In, As, Sc and V suggests that these elements partition into the same pyroxene site (M1) and share the same oxidation state (i.e., 3+).

The whole rocks element abundances were calculated by combining the contents in the minerals and the modal compositions of the peridotites in order to circumvent the problems of recent contaminations of the element budgets (e.g. by the transporting host basalt). The xenoliths define linear trends of bulk rock In, Cd and Sn with CaO respectively Yb. Using a primitive mantle value of 3.65 wt% CaO the correlations yield Earth mantle abundances of 18 ppb In, 35 ppb Cd and 92 ppb Sn, whose implication for the history of the Early Earth will be discussed.