Irreversible Thermodynamic Model for Reaction rim Growth: Application to the Forsterite-Enstatite-Quartz System

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We apply irreversible thermodynamics to model diffusion controlled growth of a reaction rim of phase γ between the mutually incompatible phases α and β in a two component system. An evolution equation is found for the system by equating the thermodynamic driving force with the dissipation associated with the irreversible processes that are operative during reaction rim growth (Svoboda et al. 2005). We allow diffusion of the two system components and the movement of phase boundaries with finite mobility as the dissipative processes. We investigate the case, where α has spherical, cylindrical and planar shape and is embedded in a matrix of β. It is shown that for non planar geometry the rim growth rate depends on the matrix-inclusion arrangement and will, in general, be different, if the α and β phases are interchanged between matrix and inclusion.
The model is applied to growth of enstatite rims at quartz-forsterite interfaces in the MgO – SiO_2 model system. Two different geometrical setups are considered, namely a spherical grain of forsterite in a quartz matrix and a spherical quartz grain in a forsterite matrix. It is shown that, for a given set of pressure-temperature conditions and for a given set of mobilities of the MgO and SiO_2 components the rim growth rate is different for the two matrix inclusion arrangements. Our model predicts an enhanced rim growth rate for the setup, where quartz is enclosed in a forsterite matrix. For enstatite rims that were grown at forsterite-quartz contacts at experimental conditions of 1000°C and 1 GPa we find that diffusion of the MgO component was rate limiting for reaction rim growth. The bulk effect of the diffusion of MgO bearing species across the poly-crystalline enstatite rim at these conditions is described by an MgO self diffusion coefficient in the range of $D_{\mathrm{MgO}} = 3*10^{-18}$ to $2*10^{-19}$ m^2/s. The effect of finite mobility of phase boundaries is expected to slow down rim growth compared to the purely diffusion controlled case. This effect is most likely relevant during the initial stages of rim growth and during rim growth in thin-film geometry, where diffusion is particularly efficient due to the short transport distances involved.
References
Svoboda J, Turek I, Fischer F (2005) Application of thermodynamic extremum principle to modeling of thermodynamic processes in material sciences. Philos. Mag. *85*: 3699-3707

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Abs. No. **14**
Meeting: **DMG 2008**
submitted by: **Abart, Rainer**
email: **abart@zedat.fu-berlin.de**
date: **2008-05-20**
Req. presentation: **Poster**
Req. session: **S09**