Summary of "Viscous constitutive relations of solid-liquid composites in terms of grain boundary contiguity, 1, 2 & 3" by Yasuko Takei & Benjamin Holtzman

Our collaboration has resulted in a series of three papers on a new model for grain boundary-diffusion creep in partially molten rocks. The broad aim is to better understand the physical processes controlling the interactions of deformation, melt distribution and melt migration. Towards this aim, we saw the need for a 3-D, grain-scale model for viscosity in the presence of melt. The constitutive relations resulting from this model enable us to study dynamic processes at longer length scales, based on micro- and meso-scale textures observed in experimental samples and natural rocks. In this model, grain scale melt geometry is described by grain boundary contiguity. Contiguity is the fraction of the total grain area that is in contact with neighboring grains, and is a useful structural state variable for describing granular media. It can be quantitatively related to melt fraction for specified values of surface energies, for texturally equilibrated materials (e.g. Takei, 2002). This geometric basis is the same as the contiguity model for homogenization of elastic properties of partially molten rocks (Takei, 1998). Thus, the viscous model is an extension of the elastic contiguity model and builds on the original work of Cooper & Kohlstedt (1984) and Cooper et al. (1989) for grain boundary diffusion creep, referred to below as the CK model. In an ab initio approach, we derived viscous constitutive relations by solving the mass and mechanical balances and reaction and diffusion kinetics for each grain, with boundary conditions determined by the 3-D distribution of grain boundary contiguity. The many questions and findings that emerged in the process of developing the model have taken the form of these three companion papers. The first focuses on the general model and its potential applications, the second on the creep behavior at very small melt fractions, and the third on the causes and consequences of viscous anisotropy.

TH1, "Grain boundary diffusion control model": The contiguity-based approach demonstrates that the 3-D pathways for matter diffusion through grain boundaries and melt, as illustrated in Fig 1a, are critical for understanding the nature of diffusion creep in partially molten rocks. The solution predicts that as long as melt forms connected pathways, matter will take the shortest path through the grain boundary, maximizing the path length through melt pockets. This model leads to several interesting results.

1) When plotted as a function of contiguity and compared to the contiguity-based model for elasticity, viscosity is more sensitive to contiguity than elasticity (Figure 1b), because of the strong dependence of viscosity on diffusion length. We also show that viscosity is more sensitive to microstructural anisotropy than elasticity. This ability of our model to calculate elastic and viscous properties from the same geometric basis will be useful for mapping between measurements or predictions of seismic properties and effective viscosity of partially molten regions of the Earth, discussed further below.

2) When plotted as a function of melt fraction (for a range of relationships between contiguity and melt fraction), the slope is similar to that of the experimentally determined dependence of viscosity on melt fraction (i.e. $\eta \sim \exp(-\lambda\phi)$), between melt fractions phi $\sim 0.005 - 0.1$, as shown in Figure 1c. Also, bulk and shear viscosity are predicted to be quite similar, with parallel slopes, a subject of importance for magma dynamics theory. The relative behavior of bulk and shear viscosity at small melt fractions is addressed in TH2.

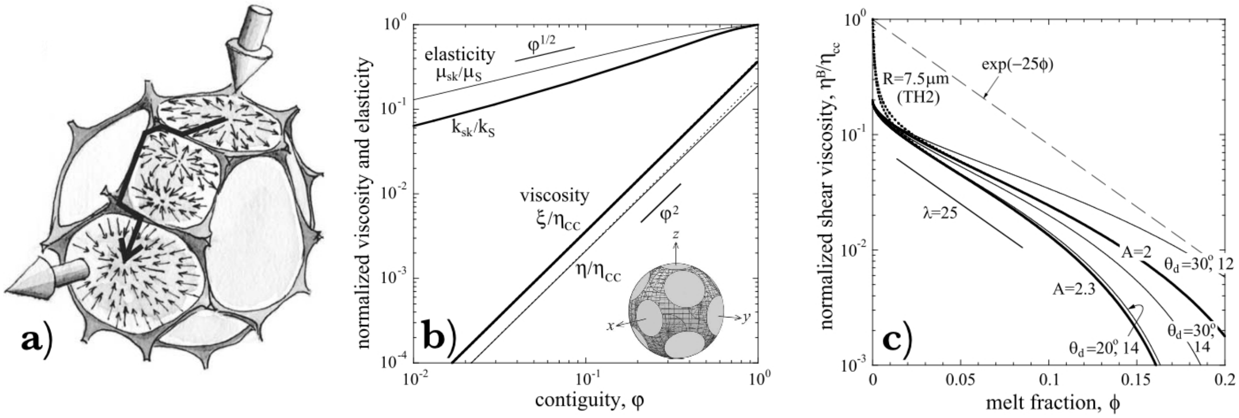

Figure 1: **From TH1: a)** A schematic illustration of a result of the contiguity model, that in 3D, matter diffusing from grain boundaries under compression to grain boundaries under relative tension will take the shortest path to the melt and the longest path within the melt tubules. **b)** Results for isotropic shear and bulk elastic and viscous properties as functions of contiguity. Inset shows the 3-D geometric basis for contiguity. **c)** Viscosity as a function of melt fraction for various relationships between melt fraction and contiguity. The dotted line at low melt fraction shows the solution from TH2, that effectively smoothes the singularity at zero melt fraction in the grain boundary diffusion control model. Also, the $\lambda = 25$ line shows the empirical fit to experimental data, with which our model is consistent.

3) The model predicts a singularity at zero melt fraction that is about a factor of 5 lower than the melt-free reference viscosity. In the grain boundary diffusion control model, this singularity is due to the simplifying assumption that melt diffusivity is infinitely high. Thus the flux in the melt is not limited, even at infinitesimally small melt fraction. Because the singularity, indicating a significant effect of very small amount of melt on viscosity, has important geological implications, we further refined the model to predict the detailed behavior of viscosity at nearly zero melt fraction, which is the subject of TH2.

TH2, "Compositional model for small melt fractions": The physical interpretation of the singularity at zero melt fraction in the diffusion control model is developed by describing the processes that occur at the microscopic scale as triple-junction tubules become infinitesimally small. While the grain boundary diffusion control model explored in TH1 assumes that melt diffusivity and reaction rates are infinitely high, the "compositional" model developed here treats finite melt diffusivity and finite reaction rates. This refinement of the model requires to specify the chemical and thermodynamic heterogeneity of melt in the system subjected to a differential stress by solving the mass balance and reaction and diffusion kinetics in the melt phase (as illustrated in Fig. 2a,b). Importantly, this model removes singularity at zero melt fraction in the grain boundary diffusion control model, as shown in Figure 1c (and 2c). The singularity is smoothed because the rate-limiting process changes from the diffusion though grain boundary to the diffusion through melt as the cross-sectional area of the pores decreases. Viscosity increases rapidly as melt fraction drops below a critical value (ϕ_c). In the mantle, this ϕ_c is predicted to be ~ 0.0001; in experimental conditions, $\phi_c \sim 0.02$. This sharp change in viscosity could help explain the large fraction

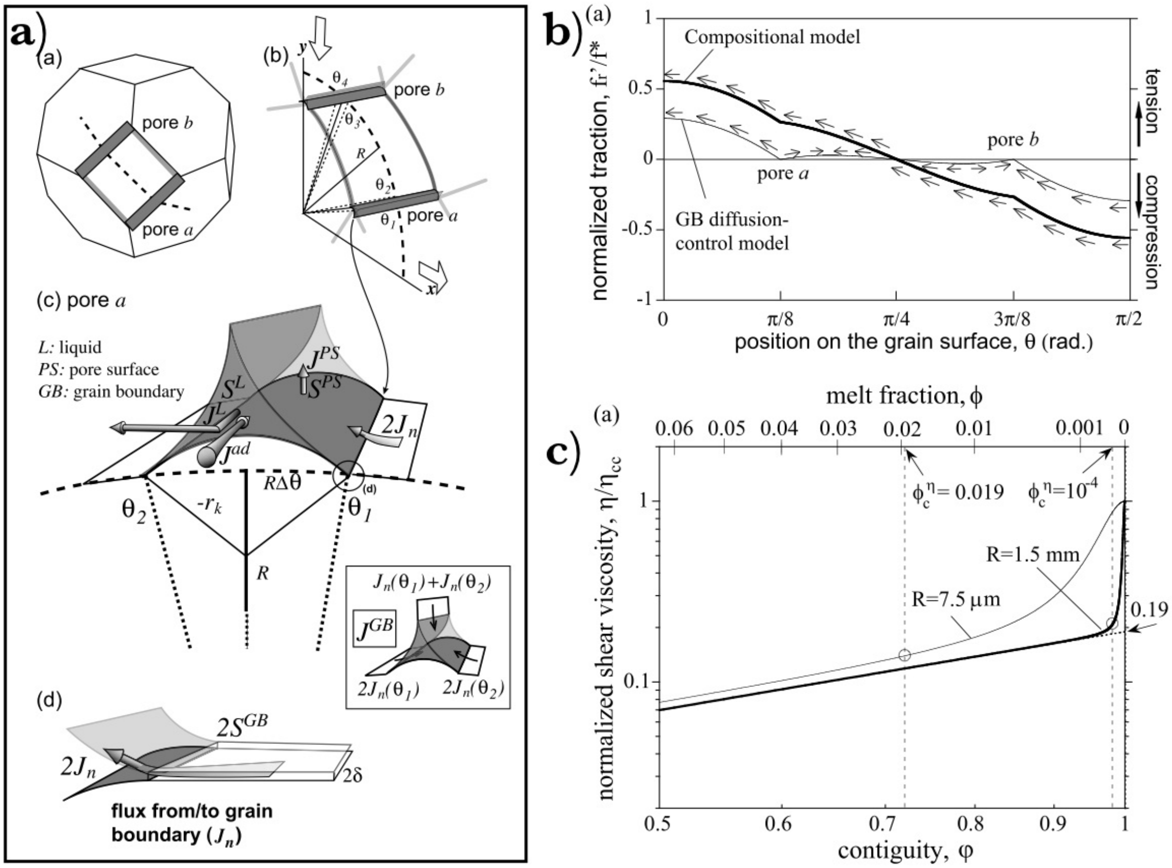

Figure 2: **Figure 2. From TH2: a)** Illustration of the model geometry and fluxes in the melt phase considered in the composition model for small melt fractions. **b)** Tractions on the 1-D (1/4 circular) grain surface for near-zero melt fraction, for the GB diffusion control model and the compositional model. The difference between the two models shown here corresponds to the presence and absence of the singularity at zero melt fraction. Arrows show the flux directions of matter. **c)** Solutions for shear viscosity as a function of contiguity for the compositional model at two different grain sizes, approximating earth- and experimental conditions.

of the differences in creep strength between "nominally" melt-free olivine aggregates (i.e. Hirth & Kohlstedt, 1995a,b) and truly melt free aggregates of synthetic olivine (i.e. Faul & Jackson, 2007). The model also predicts that ϕ_c for bulk viscosity is smaller than that for shear viscosity and bulk viscosity rapidly increases to infinite below ϕ_c. The compositional model further predicts the heterogeneous pore geometry under stress, which could establish the initial conditions for the growth of anisotropic melt distribution at the grain scale during deformation, the theme of TH3.

TH3, "Causes and consequences of viscous anisotropy": In TH1, the effects of a simple form of anisotropic contiguity on elastic and viscous properties were demonstrated. In this paper, a range of anisotropic melt distributions (or tensorial values of contiguity) were explored, designed to correspond to experimental observations of melt distribution under applied deviatoric stress (i.e. Takei, 2001, 2009; Zimmerman et al., 1999), in which melt pockets align at 0-25

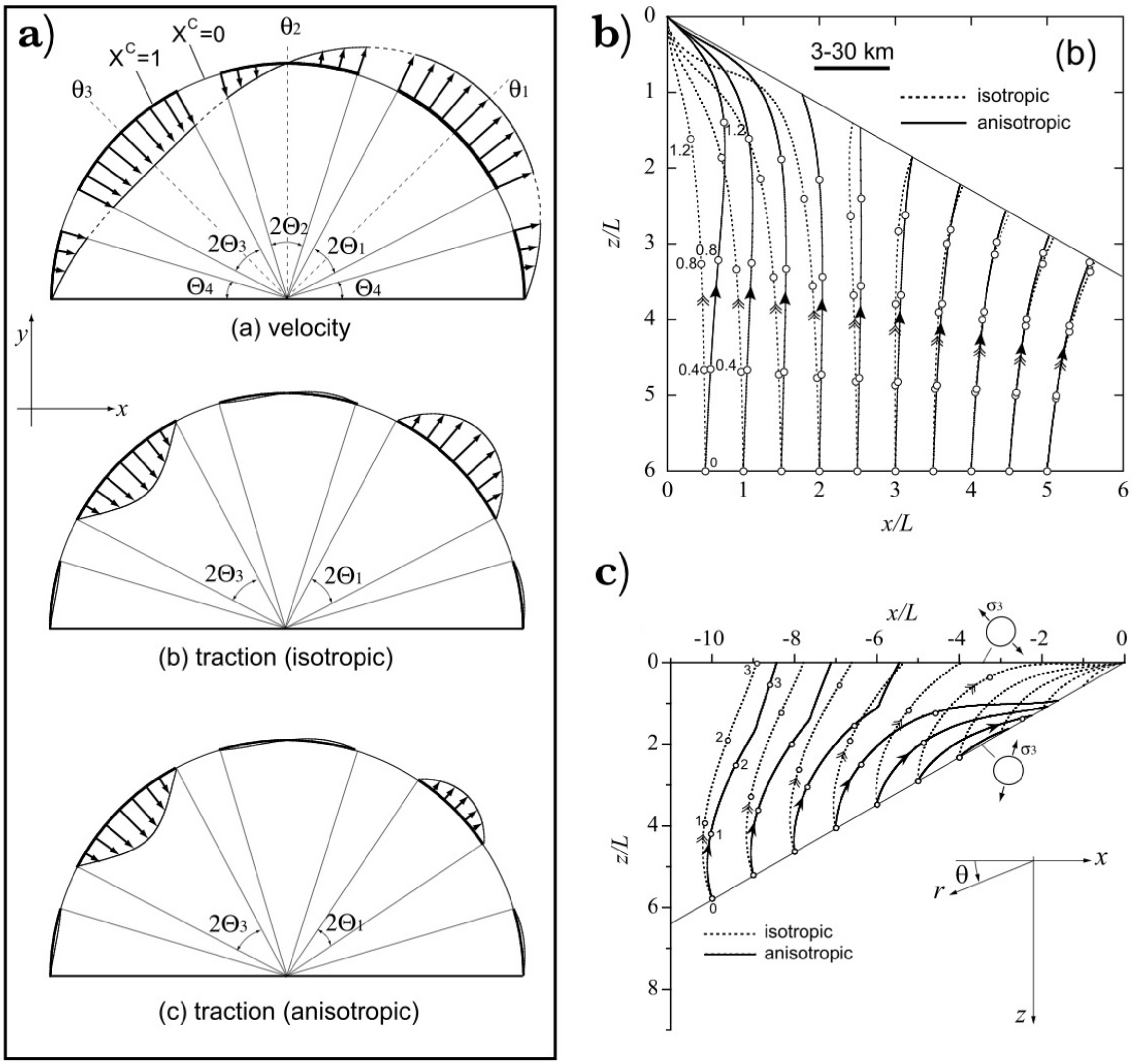

Figure 3: **Figure 3. From TH3: a)** Instantaneous velocity of grain surfaces due to deformation imposed upon a 2-D half-grain. Xc is the contact function, which equals 0 where the surface touches melt and 1 where it is a grain boundary. The middle figure shows the resulting tractions for isotropic melt/contiguity distribution, followed by that for a grain with an anisotropic melt/contiguity distribution. The asymmetry in the traction leads to a coupling between shear and isotropic components of the stress tensor. **b)** The melt flow trajectories calculated for a passive mid-ocean ridge flow for isotropic and anisotropic viscosity. The difference is due to the suction force towards regions of elevated shear stress, due to coupling between shear and isotropic components of the stress tensor (i.e. melt migration up stress gradients in the solid). **c)** Melt flow trajectories calculated for the mantle wedge of a subduction zone, for isotropic and anisotropic.

degrees to the principal compressive stress direction. Under these forms of anisotropy (with an obliquity relative to the shear plane), the anisotropic viscosity tensor causes a softening in the least compressive stress direction (σ_3), which leads to a coupling between the shear and isotropic components of the stress tensor, as illustrated in Figure 3a. This coupling has very interesting consequences for meso- and macroscopic dynamics of melt migration, explored in forward models of the macroscopic two-phase flow equations. First it predicts that melt can migrate up stress gradients in the solid matrix, as observed in experiments on solidifying metals (Gourlay & Dahle, 2005). Second, it predicts that this coupling can enhance the driving force for the segregation of melt into bands, as observed in experiments (e.g. Holtzman & Kohlstedt, 2007), and stabilize those bands at low angles to the shear plane (without a stress exponent greater than unity, e.g. Katz et al., 2006). Finally, it predicts that in geodynamic settings, melt will be attracted to the regions of highest shear stress. In a mid-ocean ridge, this region forms a lobe pointing towards the ridge axis, dipping 45 degrees (Fig. 3b); in a subduction zone corner flow, this suction effect will keep melt or fluid focused along the top of the slab (Fig. 3c). Melt migration to these interfaces will enhance the reduction of effective viscosity, causing a lubrication effect at a geodynamic scale.

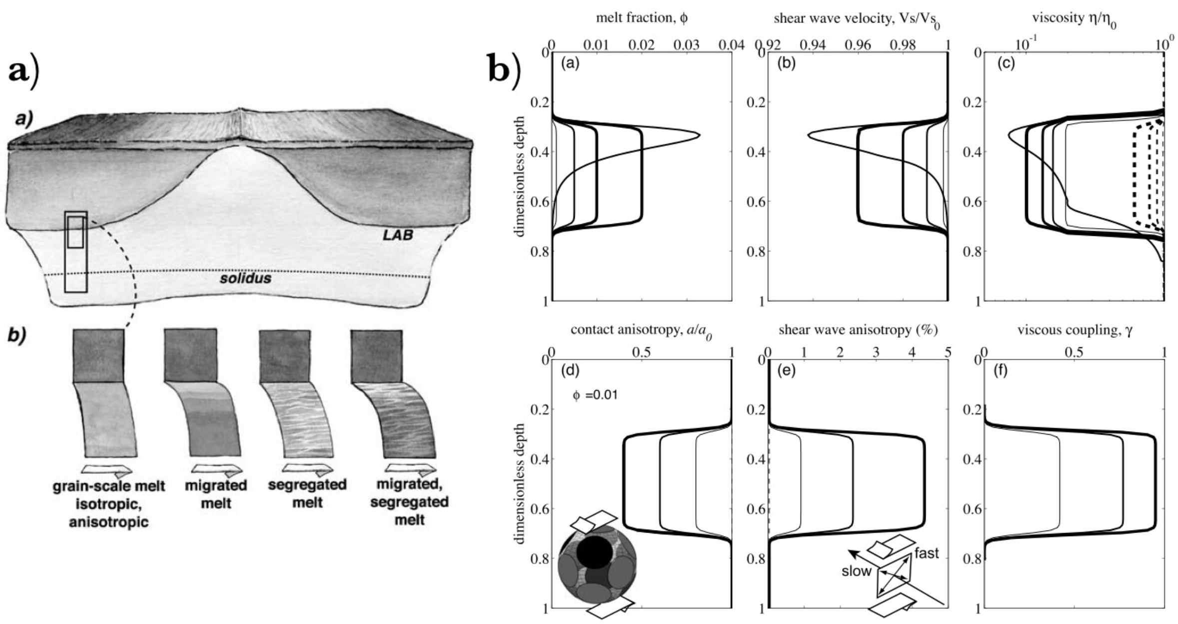

Figure 4: **Applications to Earth, from TH1: a)** Schematic illustration of a mid-ocean ridge and a suite of hypothetical melt distributions beneath the plate. **b)Top row:** hypothetical isotropic melt fraction distributions beneath the plate, and resulting shear wave velocity reduction and corresponding viscosity reduction. The dashed lines represent the empirical relation from experiments on melt-bearing samples. The difference between the empirical curves and model predictions indicates the potential importance of the difference between nominally melt-free and truly melt-free rocks, discussed in TH2. **Bottom row:** hypothetical distributions of contact anisotropy in the contiguity model, resulting shear wave anisotropy and degree of viscous coupling between the shear and isotropic parts of the stress tensor.

Applications to Earth: In TH1, we demonstrated a simple approach to the application of this contiguity model to upper mantle situations, namely the base of an oceanic plate, by forward modeling the effects of various melt-distribution profiles on viscous and elastic properties (Fig 4a,b). The first direct application of this model to seismic observations was recently published in Kawakatsu et al., 2009. They detected large amplitudes of P-to-S and S-to-P converted waves, indicating a 7-8% contrast in shear wave velocity at the base of oceanic plates in the western Pacific. The contiguity model was used to calculate the velocity contrast and the corresponding viscosity contrast at the lithosphere-asthenosphere boundary. A range of solutions for different melt fractions and distributions were calculated, from a homogeneous partially molten asthenosphere to a multi-scale layered model consisting of horizontal melt-rich and melt-free layers. The multi-scale model, but not the homogeneous model, is consistent with several diverse constraints, 1) the observed large velocity contrast from receiver functions, 2) dynamical models of plate-mantle interactions that indicate a need for a large viscosity constrast (10^3) across the LAB (e.g. Hoeink & Lenardic, 2008; Takaku & Fukao, 2008) 3) geochemical studies that indicate only a small melt fraction ($< 1\%$) resides within the asthenosphere (references within Kawakatsu et al., 2009). While there is much yet to learn, mapping from seismic velocity measurements to viscosity estimates is becoming possible. As we began to explore in TH3, the contiguity model also enables us to simulate the formation of such multi-scale structures based on microstructural processes.

References

Cooper, R., D.L. Kohlstedt and K. Chyung. Solution-precipitation enhanced creep in solid-liquid aggregates which display a non-zero dihedral angle. Acta Metall Mater (1989) vol. 37 (7) pp. 1759-1771.

Faul, U. and I. Jackson. Diffusion creep of dry, melt-free olivine. J. Geophys. Res. (2007) vol. 112 (B4) pp. 14

Gourlay, C. and A. Dahle. Shear deformation at 29% solid during solidification of magnesium alloy AZ91 and aluminium alloy A356. Materials Science and Engineering: A (2005) vol. 413-414 pp. 180-185

Hirth, G. and D. L. Kohlstedt. Experimental constraints on the dynamics of the partially molten upper mantle: Deformation in the diffusion creep regime. J. Geophys. Res. (1995) vol. 100 (B1) pp. 1981-2001

Hoeink, T. and A. Lenardic. Three-dimensional mantle convection simulations with a low-viscosity asthenosphere and the relationship between heat flow and the horizontal length scale of convection. Geophys Res Lett (2008) vol. 35 (10)

Holtzman, B. and D. L. Kohlstedt. Stress-driven Melt Segregation and Strain Partitioning in Partially Molten Rocks: Effects of Stress and Strain. Journal of Petrology (2007) vol. 48 (12) pp. 2379-2406

Katz, R., M. Speigelman, B. Holtzman. The dynamics of melt and shear localization in partially molten aggregates. Nature (2006) vol. 442 (7103) pp. 676-679

Kawakatsu, H., P Kumar, Y Takei, M Shinohara, T Kanazawa, E Araki, and K Suyehiro. Seismic evidence for Sharp Lithosphere-Asthenosphere Boundaries of Oceanic Plates. Science (2009) vol. 324 pp. 499

Takaku, M. and Y. Fukao. Fluid mechanical representation of plate boundaries in mantle convection modeling. Physics of The Earth and Planetary Interiors (2008) vol. 166 (1-2) pp. 44-56

Takei, Y. and B. Holtzman. Viscous constitutive relations of solid-liquid composites in terms of grain boundary contiguity: 1. Grain boundary diffusion control model. J. Geophys. Res. (2009) vol. 114 (B6) pp. 19

Takei, Y. and B. Holtzman. Viscous constitutive relations of solid-liquid composites in terms of grain boundary contiguity: 2. Compositional model for small melt fractions. J. Geophys. Res. (2009) vol. 114 (B6) pp. 18

Takei, Y. and B. Holtzman. Viscous constitutive relations of solid-liquid composites in terms of grain boundary contiguity: 3. Causes and consequences of viscous anisotropy. J. Geophys. Res. (2009) vol. 114 (B6) pp. 23

Takei, Y. Stress-induced anisotropy of partially molten media inferred from experimental deformation of a simple binary system under acoustic monitoring. J. Geophys. Res. (2001) vol. 106 (B1) pp. 567-588

Takei, Y. Deformation-induced grain boundary wetting and its effects on the acoustic and rheological properties of partially molten rock analogue. J. Geophys. Res. (2005) vol. 110 (B12) pp. 24

Takei, Y. Stress-induced anisotropy of partially molten rock analogue deformed under quasi-static loading test, J. Geophys. Res. (2009), doi:10.1029/2009JB006568, in press.

Takei, Y. Constitutive mechanical relations of solid-liquid composites in terms of grain-boundary contiguity. J. Geophys. Res. (1998) vol. 103 (B8) pp. 18,183-18,203

Zimmerman, ME., SQ Zhang, DL Kohlstedt, S Karato. Melt distribution in mantle rocks deformed in shear. Geophys. Res. Lett. (1999) vol. 26 (10) pp. 1505-1508