PROJECT PLAN

Results from prior NSF support

Karato, S. (PI), "Deformation of transition zone minerals" EAR-9805217 (8/1/98-7/31/01), $350,000

We have investigated the rheology of germanate spinels in detail. We first synthesized germanate spinel with Ni2GeO4 and Fe2GeO4 at room pressure and high temperatures. Deformation experiments were conducted using the gas apparatus. The results show deformation by either dislocation and diffusion creep regimes. Flow laws were determined in each regime. A comparison of these results with those on other spinels indicates that germanate spinels and a stoichiometric MgAl2O4 spinel form an isomechanical group. We have also prepared olivine-spinel mixtures of (Mg,Ni)2GeO4 by the synthesis at relatively low pressures (¡300 MPa). In these samples, the volume fraction of olivine can be changed by changing the pressure or temperature in the P-T range that is realizable in the Paterson gas apparatus. This allows us to conduct high resolution mechanical tests during the olivine-spinel transformation. Our initial results at 1300 K and 300 MPa showed that transformational superplasticity proposed by some previous works does not work for this system under these conditions.

The new technique of ultrahigh pressure deformation developed by *Karato and Rubie* (1997) has been used to deform spinel and modified spinel phases of (Mg,Fe)2SiO4 (ringwoodite, wadsleyite) as well as ilmenite phase of (Mg,Fe)SiO3 (e.g., *Karato et al.,* 1998a). During the summer of 1998 and 1999, we have developed a new sample assembly of two-layer shear deformation has been tested successfully for the first time. In this assembly, two samples with different chemistry or different grain-sizes are deformed at exactly the same conditions. After a deformation experiment, we can determine the strains in each layer by measuring the angles of strain markers. This provides us with a precise data on the relative strength of two samples. We have applied this technique to two types of samples: a pair of olivine and wadsleyite with slightly different Fe content and wadsleyite with different grain-sizes.

Karato, S. (PI) "Effects of water and deformation history on the development of lattice preferred orientation in olivine-rich rocks" EAR-9706329 (9/97-8/99), EAR-9903087 (8/1/99-7/31/2002), $288,000

We have installed an Electron BackScattered Pattern (EBSP) facility to measure LPO. We investigated the role of dynamic recrystallization on LPO in olivine under relatively water-poor conditions. Samples used were deformed in simple shear using the Paterson apparatus at relatively water-poor conditions (300 MPa, 1473 - 1573 K). Using EBSP, one can determine the orientations of small (recrystallized) grains separately from those of large (host) grains. Our results clearly demonstrate that the orientations of these two groups of grains are different. We are currently investigating the cause of this difference by combining EBSP with SEM and TEM observations of dislocations.

We have also started the study of effects of water on LPO in olivine. Synthetic olivine aggregates were deformed in simple shear mode using the Griggs apparatus to 2 GPa confining pressure at 1473 K and strain-rate of 10-4 s-1. Water was added by the dehydration of talc + brucite. The FT-IR measurements of samples after experiments showed that they were saturated with water under the experimental conditions. Under these conditions, the fugacity of water is 30-100 times higher than that at 300 MPa confining pressure. Deformation experiments were made to 100 and 200Samples deformed under water-rich conditions showed

LPO which is totally different from those deformed water-poor conditions. Olivine [001] axis is aligned nearly parallel or about 30-40o with respect to the flow direction and olivine (100) plane is nearly parallel to or 30-40o inclined with respect to the flow plane. This result has important implications for deep upper mantle anisotropy in water-rich regions.

Selected Publications

1. Jin, D., Karato, S. and Obata, M., Mechanisms of shear localization in the continental lithosphere: Inference from deformation microstructures of peridotites from the Ivrea zone, northwestern Italy, J. Struct. Geol., 20; 195-209 (1998).
2. Jung, H. and Karato, S., Water-induced fabric transition in olivine, submitted to Science.
3. Karato, S., Phase transformations and rheological properties of mantle minerals, In Earth's Deep Interior (eds. D. Crossley and A.M. Soward), Gordon and Breach, pp. 223-271 (1997).
4. Karato, S., Seismic anisotropy in the deep mantle, boundary layers and the geometry of mantle convection, PAGEOPH, 151: 565-587 (1998a).
5. Karato, S., Some remarks on the origin of seismic anisotropy in the D" layer, Earth, Planets and Space, , 50: 1019-1028 (1998b).
6. Karato, S., A dislocation model of seismic wave attenuation and micro-creep in the Earth: Harold Jeffreys and the rheology of the Earth, PAGEOPH, 153: 239-256 (1998c).
7. Karato, S., Effects of high pressure on plastic deformation of polycrystalline solids: Some geological applications, in High Pressure Research in Materials Sciences", Materials Research Society, pp. 3-14 (1998d).
8. Karato, S., Seismic anisotropy of Earth's inner core caused by flow induced by the Maxwell stress, Nature, 402: 871-873 (1999).
9. Karato, S. and Jung, H., Partial melting, water and the origin of the seismic low velocity zone, Earth Planet Sci. Lett. , 157: 193-207 (1998).
10. Karato, S. and Rubie, D.C., Toward an experimental study of deep mantle rheology: a new multi-anvil specimen assembly for deformation experiments under high pressures and temperatures, J. Geophys. Res. , 102: 20,111-20122 (1997).
11. Karato, S. and Karki, B., Origin of velocity heterogeneity in the Earth's mantle, submitted to J. Geophys. Res.
12. Yamazaki, D. and Karato, S., Some mineral physics constraints on the rheology of Earth's lower mantle, submitted to Phys. Earth Planet. Inter.
13. Karato, S., Zhang, S. and Wenk, H-R., Superplasticity in the lower mantle: evidence from seismology and mineral physics, Science, 270: 458-461 (1995a).
14. Karato, S., Wang, Z., Liu, B. and Fujino, K., Plastic deformation of garnets: systematics and implications for the rheology of the mantle transition zone, Earth Planet Sci. Lett., 130: 13-30 (1995b).
15. Karato, S., Dupas-Bruzek, C. and Rubie, D.C., Plastic deformation of (Mg,Fe)2SiO4 spinel (ringwoodite) under the transition conditions of the Earth's mantle, Nature, 395: 266-269. (1998).
16. Karato, S., Zhang, S., Zimmerman, M.E., Daines, M.J. and Kohlstedt, D.L., Shear deformation of mantle materials, PAGEOPH , 151: 589-603 (1998c).
17. Li, P., Karato, S. and Wang, Z., High temperature creep of fine-grained CaTiO3 perovskite, Phys. Earth Planet. Inter., 95: 19-36 (1996).

18. Riedel, M.R. and Karato, S., Grain-size evolution in subducted oceanic lithosphere associated with the olivine-spinel transformation and its effects on rheological weakening, Earth Planet. Sci. Lett., 148: 27-44 (1997).
19. Zhang, S. and Karato, S., Preferred orientation of olivine deformed in simple shear, Nature, 375: 774-777 (1995).
20. Zhang, S. and Karato, S. and Zhou, Y., Simple shear deformation of olivine, Tectonophysics in press.
21. Zimmerman, M.R., Zhang, S., Kohlstedt, D.L. and Karato, S., Melt distribution in mantle rocks deformed under shear conditions, Geophys Res. Lett. 26: 1505-1508 (1999).

B.Romanowicz (P.I.) "3D mapping of attenuation in the mantle" EAR-9405927 (09/15/94-06/30/98), $203,000; **"Global attenuation model of the whole mantle using waveform tomography"** EAR-9706380 (09/01/97-12/31/99), $140,000

We have developed a waveform inversion approach based on normal mode summation for the determination of mantle elastic and anelastic structure. Whole mantle, 3D SH velocity models have been obtained using surface and body waveforms as well as $NACT$ theory (Non-linear asymptotic coupling theory, Li and Romanowicz, 1995, 1996), which allows the computation of accurate 2D kernels for body waves, and have attained progressively higher lateral resolution : degree 12 for SAW12D (Li and Romanowicz, 1996), degree 24 for SAW24B16 (*Mégnin and Romanowicz,* 1999). We have extended the elastic inversion to an iterative procedure for elastic as well as anelastic structure, so far applied successfully to the upper mantle (*Romanowicz,* 1997, *Gung and Romanowicz,* 1999), building upon our previous experience with frequency domain, surface wave inversions for 3D Q (*Romanowicz,* 1995; *Romanowicz,* 1998; *Romanowicz and Durek,* 2000). Indeed, we have inverted transverse component waveforms (fundamental and higher mode Love wave data) in the period range 80-300 sec for a 4 layer model of Q_β in the upper mantle, using as starting model for elastic velocities, the degree 12 SH velocity model SAW12D (*Li and Romanowicz,* 1996) and model QL6 (*Durek and Ekstrom,* 1995), as starting, radially symmetric Q model. The waveforms were corrected for effect of earthquake sources, applying perturbations to CMT solutions obtained during the construction of model SAW12D. In order to obtain a stable 3D Q model, it was necessary to apply a strict selection criterion to the data, based on the comparison of observed and synthetic seismograms, the latter computed in the model SAW12D, for each wave-packet considered. Only those waveforms were kept which satisfied an rms residual with respect to the syntethic of < 0.75. This reduced the number of waveforms considered by about a half, compared to the dataset used for elastic inversions, and resulted in a reduction in sampling and lateral resolution. Nevertheless, the "degree 5" Q model obtained for the upper mantle is in good qualitative agreement with that obtained previously in Romanowicz(1995) even though both the type of data (transverse versus vertical component) and method (time domain versus frequency domain) are completely different.

Selected publications and presentations

Gung and Romanowicz (1999) Q tomography of the Earth using long period waveform data, EOS Trans AGU, 80, F733.
Li, X-D and Romanowicz, B., 1995. Comparison of global waveform inversions with and without considering cross-branch modal coupling, Geophys. J. Int., 121, 695-709.

Li, X-D and Romanowicz, B., 1996. Global mantle model developed using nonlinear asymptotic coupling theory, J. Geophys. Res., 101: 22,245-22,272.
Mégnin, C. and B. Romanowicz (1999) The 3D shear velocity structure of the mantle from the inversion of body, surfave, and higher mode waveforms, submitted to Geophys. J. Int.
Romanowicz, B. (1994a) On the measurement of anelastic attenuation using amplitudes of low frequency surface waves, Phys. Earth Planet. Int., 84, 179-191.
Romanowicz, B. (1994b) Anelastic tomography: a new perspective on upper-mantle thermal structure, Earth. Planet. Sci. Lett., 128, 113-121.
Romanowicz, B. (1995) A global tomographic model of shear attenuation in the upper mantle, J. Geophys. Res., 100, 12,375-12, 394.
Romanowicz, B. (1997) 3D models of elastic and anelastic structure in the mantle, EOS Trans AGU, 78, F466.
Romanowicz, B. (1998) Attenuation tomography of the Earth's Mantle: a review of current status, Pageoph.,153, 257-272.
Romanowicz, B. and J. Durek (2000) Seismological constraints on attenuation in the earth: a review, AGU Monograph, in press.

PROPOSED WORK: Introduction

Heterogeneity in physical properties and chemical composition reflects current dynamic processes and chemical evolution in the earth's interior. In this collaborative research, we focus on the upper mantle (down to 670 km depth), where the largest lateral variations in elastic and anelastic properties have been observed, likely to be due to large lateral variations in temperature and chemical composition. For these regions, three-dimensional elastic and anelastic structure can be revealed from seismology on the global scale. A reasonably well-established mineral physics dataset on elasticity and anelasticity is also available, particularly for the upper mantle above the 410 km discontinuity (*Anderson et al.,* 1992; *Jackson et al.,* 1992; *Jackson,* 2000;*Karato,* 1993; *Karato and Karki,* 2000).

A dynamic and evolving planet like the earth is expected to have heterogeneity in both chemical composition and temperature. The effects of changes in major element composition on elastic properties and density have been known and incorporated into some previous models of composition of Earth's upper mantle (e.g., *Jordan,* 1975, 1979). Fe depletion and a large content in Ca and Al result in an increase in seismic wave velocity but a decrease in density. In addition to these well known effects of major elements, recent studies have shown that minor elements such as H (hydrogen) can dramatically change seismic wave velocities and attenuation (Karato, 1995; Karato and Jung, 1998). Petrological studies of processes of partial melting indicate that composition of both major (Fe, Ca and Al, for example) and minor (e.g., H) elements should be modified by partial melting which has formed various volcanic rocks including MORB (mid-ocean ridge basalts) and komatiite (e.g., *Takahashi*, 1986, 1990, 1997). Takahashi (1997) reviewed petrological observations on upper mantle rocks and concluded that the Archean continental upper mantle has significantly lower Fe content than those in the source regions of MORB. He argued that the old continental upper mantle had undergone partial melting at high temperatures involving Mg- rich komatiite magmas resulting in a higher degree of partial melting than in the case involving MORB. Partial melting in a water-undersaturated mantle results in water depletion in a residual mantle (*Karato,* 1986; *Hirth* *and Kohlstedt,* 1996; *Karato and Jung,* 1998). Therefore in evaluating variation in chemical composition from seismological observations, one needs to consider the effects of both major element and water. Both temperature and chemical composition affect rheological properties that control the dynamics of Earth's interior. Temperature effects on rheology are well known. Effects of major element composition on rheology can be inferred, and turn out to be relatively small: the viscosity of an upper mantle rock will change by $\sim 4-10\%$ as a result of change in Fe content of 2-5%. In contrast, the effects of change in water content can be large: viscosity can vary between water-poor and water-rich environment by as much as a factor of ~ 100 (*Karato et al.,* 1986; *Hirth and Kohlstedt,* 1996). Thus, estimating lateral variations in temperature, chemical composition and water content is critical to our understanding of the dynamics of the earth's upper mantle.

Through the mapping of 3D variations in elastic velocities and attenuation in the deep mantle, global seismic tomography gives us indirect access to key parameters for the understanding of global mantle dynamics. Starting from seismological data, we are therefore faced with two challenges: 1) to resolve the variations in the seismic parameters accurately, and 2) to interpret the latter using insights gained from theoretical and experimental mineral physics.

Elastic tomography has progressed faster than anelastic tomography, because it uses the information contained in the phase, or travel-time, which is relatively unaffected by other factors besides the seismic velocity distribution along the wave travel path. Anelastic tomography should provide a more direct access to temperature, however, seismic amplitudes, which are needed to measure attenuation, are strongly affected by many perturbing effects, such as scattering and focusing.

In what follows, we first review the status of global elastic and anelastic tomography, discuss the major issues facing the latter and how they have been dealt with so far, and review the available results from mineral physics. We then proceed to describe a methodology in which we propose to invert long period seismic waveform data *directly* for lateral variations in temperature and composition in the deep upper mantle and through the transition zone. This cooperative work between seismologists and mineral physicists will combine the expertise of the former in seismic waveform inversions and that of the latter in devising the appropriate parametrization of the target 3D model, and in interpreting the resulting distributions.

Current status of elastic and anelastic tomography

Global elastic tomography has made great strides since the pioneering studies of the last two decades (*Dziewonski et al.,* 1977; *Woodhouse and Dziewonski,* 1984, *Nataf et al.,* 1986). It is currently possible to resolve whole mantle S velocity structure at degree 12 with reasonable agreement between different studies (*Su et al.,* 1994; *Li and Romanowicz,* 1996; *Masters et al.,* 1996) and upper mantle structure with even greater detail, with lateral resolution reaching on the order of 500-1000 km (*Montagner and Tanimoto,* 1991; *Ekstrom et al.,* 1997; *Laske and Masters,* 1996; *Trampert and Woodhouse,* 1996). Such a resolution is also progressively attainable in the lower mantle, both for S and P velocities (*Vasco et al.,* 1995; *Grand et al.,* 1997; *vanderHilst et al.,* 1997; *Masters et al.,* 1999; *Megnin and Romanowicz,* 1999). Comparison of S and P velocity distributions have, in particular, revealed an increase in the S/P velocity ratio in the deep mantle that is difficult to explain by temperature variations alone (e.g. *Robertson and Woodhouse,* 1995; *Su and Dziewonski,* 1997; Bolton et al., 1996).

In contrast, resolving lateral variations of attenuation in the deep mantle by tomographic methods is a challenging subject which has been addressed by only a few studies until now. Nevertheless, the existence of large lateral variations of Q in the crust (see *Mitchell,* 1995 for a review) and the uppermost mantle is well documented from various regional studies either using surface waves (e.g. *Mitchell,* 1975; *Canas and Mitchell,* 1978, 1981; *Nakanishi,* 1979a; *Bussy et al.,* 1993) or body waves, such as multiple ScS phases (*Nakanishi,* 1979b; *Sipkin and Jordan,* 1980; *Lay and Wallace,* 1983; *Chan and Der,* 1988; *Sipkin and Revenaugh,* 1994) or multiple S and depth phases (*Sheehan and Solomon,* 1992; *Flanaghan and Wiens,* 1990; 1994;*Ding and Grand,* 1993). These lateral variations can be an order of magnitude larger than observed lateral variations in velocity, commonly exceeding 50-100%.

At greater depth, even though the degree 2 pattern in Q in the upper mantle is not as prominent as that of elastic velocities in studies of free oscillations and surface waves *(Smith and Masters,* 1989), it appears to be reasonably well constrained (*Romanowicz et al,* 1987; *Roult et al.,* 1990;*Romanowicz,* 1990; *Suda et al.,* 1991; *Durek et al.,* 1993), with significant correlation between the results of surface wave and body wave studies (*Bhattacharyya et al.,* 1996). This structure is also well correlated with degree 2 in elastic velocities, and in particular shows a similar shift in phase towards the west as one goes from the uppermost mantle (first 300km) into the transition zone (400-600 km), which is indicative of the predominantly thermal nature of heterogeneity at these long wavelengths (e.g. *Montagner and Romanowicz,* 1992). Even at such long wavelengths, there is however some disagreement concerning the depth distribution of attenuation. Durek et al. (1993) argued that the lateral variations in Q are primarily confined to the depth range corresponding to the seismic low velocity zone (80-220 km), whereas more recent studies indicate significant heterogeneity persisting into the transition zone (*Romanowicz,* 1995; *Bhattacharya et al.,* 1996). In general, models obtained so far at the global scale concur with regional scale models on the existence of a correlation of lateral variations in Q with tectonic province, in the first 250 km of the upper mantle, with high Q under shields and low Q under oceans. Surface wave derived models (*Romanowicz,* 1990; 1995;*Durek et al.,* 1993) tend to indicate high attenuation under young oceans (as confirmed by regional studies, e.g. *Ding and Grand,* 1993). *Romanowicz* (1994b) showed correlation of Q with age of the sea floor in the first 250 km of the upper mantle both in the Pacific and in the Atlantic oceans. In this depth range, correlation of Q structure with heat flow is also observed. At greater depths in the south Pacific, the shift to the west of the high Q maximum observed at degree 2 also persists at shorter wavelength, perturbing the correlation with age of the sea floor. In this depth range, the correlation of Q with hotspot distribution appears to be significant (*Romanowicz,* 1994b, 1995). Regional scale Q models confirm the correlation with tectonic features such as slabs, back arc basins and different continental provinces (e.g. *Mitchell*, 1995; *Roth et al.*, 1999).

While they are often still very qualitative, the Q results confirm that the expected variations are related to the effects of temperature, and potentially fluid content. Resolution is however poor, and is especially insufficient to address such important questions as the origin of hot spots and, more generally, the detailed structure of mantle upwellings.

The quality factor Q of the earth is much more sensitive to temperature than elastic velocity, as shown by laboratory and theoretical studies (e.g. *Minster and Anderson,* 1981; *Berckhemer et al.*, 1982; *Gueguen et al.*, 1989; *Karato and Spetzler,* 1990; *Jackson et al.,* 1992) and this sensitivity is different from that of elastic velocity. As argued by *Romanowicz* (1994b), the non-linear (Arrhenius law) sensitivity of Q to temperature implies that, in principle, attenuation tomography should be able to resolve *hot* regions (high attenuation) better than elastic tomography. In addition, elastic velocity can be affected to a large degree by compositional variations (e.g. *Yan et al.,* 1989; *Bina and Silver,* 1997), so, ultimately, mapping regions with various degrees of agreement between velocity and attenuation distributions should help constrain the distribution of chemical versus thermal heterogeneity in the mantle. At shallow depths, as discussed by *Mitchell* (1995), and perhaps also near the core-mantle boundary, the effect of fluid inclusions and partial melt on attenuation also needs to be considered.

While it is easily recognized that accurately resolving 3D anelastic structure of the mantle could be very useful to further our understanding of mantle dynamics, progress has so far been slow because of the inherent difficulty of measuring attenuation and especially its lateral variations. Indeed, the amplitude of seismic waves travelling through the earth is affected not only by anelastic attenuation but also by focusing and scattering effects due to propagation in a 3D elastic medium. The latter can be as large or larger than anelastic effects and depend strongly on the short wavelength details of the elastic structure, which are at present not very well constrained. Indeed, as shown by *Woodhouse and Wong* (1984) in the framework of ray theory and by *Romanowicz and Roult* (1986), *Romanowicz* (1987) and *Park* (1987) in the framework of asymptotic normal mode theory, to first order, the focusing terms due to elastic structure depend on the transverse gradients of velocity along the propagation path. For a velocity model described by an expansion in spherical harmonics with coefficients (Clm, Slm), transverse gradients depend on terms of the form l^2Clm, l^2Slm, and are therefore sensitive to large values of l, in other words, short wavelengths.

If the elastic structure of the earth were perfectly known, one could first correct for its effects using either linear theory (Born approximation), or, preferably, a more complete formalism including multiple scattering effects (e.g. *Lognonné and Romanowicz,* 1990; *Friederich,* 1997; *Geller and Hara,* 1993). Current global 3D models are slowly becoming reliable enough at short wavelengths so that, combined with the increase in computer power, such corrections can progressively become reliable.

Until now however, indirect ways of dealing with focusing and scattering have generally been used. *Romanowicz* (1990) and *Durek et al.* (1993) exploited the fact that, for surface waves and in the case of linear theory, focusing and anelastic effects could be separated by combining measurements over several consecutive wavetrains for a single recording, because focusing terms change sign with the direction of propagation whereas attenuation terms are always additive. An alternative approach, favored by *Romanowicz* (1995) for surface waves and *Bhattacharyya et al.* (1996) for body waves, is to reject data that are strongly affected by focusing, after visual inspection. In the case of body waves, *Bhattacharyya et al.* (1996) used a technique in which the attenuation operator t* is inferred from the slope of the variation with frequency of SS to S amplitude ratios. Data for which a smooth variation of this ratio with frequency cannot be obtained are rejected. In the case of surface waves, Romanowicz (1994a) devised a technique that allows to 1) keep only data for first arriving trains that have travelled the shortest paths (e.g. R1 and R2 for Rayleigh waves), and 2) among those data, reject those that do not present a smooth variation of attenuation coefficient with period. This approach appears to work, provided very strict rejection criteria are applied, which limits the available coverage of the earth and therefore the spatial resolution of three-dimensional structure.

The published models to-date generally rely on amplitude measurements in the frequency domain. This is suitable for isolated phases, such as fundamental mode surface waves or specific body wave phases such as S, SS and ScS. More recently, we have started to explore the possibility of using time-domain waveform information to invert for anelastic structure (*Romanowicz,* 1997; *Gung and Romanowicz,* 1999), which should allow us to extend attenuation measurements to a larger portion of the seismogram, and therefore increase sampling of the deep mantle. In the case of surface waves, a time-domain method based on the comparison of observed and synthetic waveforms helps resolve the problem of contamination of fundamental modes by higher mode energy, inherent in frequency domain methods, and, more generally, the problem of length of time window considered to compute the spectrum, and the dependence of amplitudes on chosen tapers. Such an approach requires the ability to accurately account for 3D elastic structure. This approach follows the general framework of global waveform inversion for elastic structure developed by *Li and Romanowicz* (1995, 1996) and proceeds in an iterative manner: in the first step, a spherically symmetric attenuation model is assumed, and waveform data are inverted for 3D elastic structure. In the second step, the derived 3D elastic structure is used as starting model for an inversion for 3D anelastic structure. In this second step, focusing terms due to the elastic structure can be incorporated in the forward computation of seismograms. Preliminary results indicate that this approach is promising and results in models that are at least qualitatively compatible with those obtained earlier using a different dataset and a spectral approach (figure 1). This raises hope as to the feasibility of resolving finer details of Q structure in the upper mantle.

Experimental constraints on velocity and attenuation in the earth's mantle

Relevant experiments represent a considerable challenge, especially for attenuation, due to the difficulties of reproducing *both* the mantle conditions of temperature and pressure *and* the low- frequency range of seismic observations. Due to the absorption band structure of seismic observations, with a high frequency cut-off around a period of 1 sec, experiments conducted at ultrasonic frequencies (100-900 kHz), which more easily allow simultaneous high T and high P domains of experimentation, may not be extrapolated to seismic conditions. *Sato et al.* [1989] have argued that, if the dominant relaxation mechanism is related to grain boundary processes, a simple scaling law relating grain size to frequency could be applied to extrapolate their ultrasonic results (namely a dependence of Q^{-1} on homologous temperature), to the domain of seismic observations. While providing a very attractive and convenient procedure to interpret observed lateral variations of Q in the upper mantle, caution must be applied, since it is not clear at present that grain boundary processes are the primary cause of seismic attenuation, in fact, dislocation mechanisms are just as likely and appear to be favored at the present time [i.e. *Karato,* 1998]. A difficult experimental technique operating in the seismic frequency band, and involving observation of forced torsional oscillations of rock samples has been developed over the last 20 years. First conducted at ambient pressure and temperature conditions, this technique was used to demonstrate the validity of the linear (amplitude independent) regime for internal friction of rocks (e.g. Brennan, 1981). Further developments have allowed the extension of experimental conditions to lower-crust/upper-mantle temperatures (1200-1500K) (Berckhemer et al., 1982; Gueguen et al.,1989; Kampfmann and Berckhemer, 1985) or pressures (0.3 Gpa) (Jackson et al., 1984; Jackson and Patterson, 1987). It is only recently that both relatively high temperature (1000^oC) and high pressure (0.3 GPa) have been achieved simultaneously (Jackson et al., 1992), and have confirmed the amplitude independence of Q^{-1} for mantle relevant strains ($< 10^{-6}$). The experimental technique involves the measurement of strain amplitude and phase resulting from a sinusoidally applied stress. Its detailed description and a review of current status is given in Jackson (1993). Experimental results find a frequency dependence of Q^{-1} of the form:

$$Q^{-1}(\omega, T) = B\omega^{-\alpha} exp(-\alpha H^*/RT) \tag{1}$$

where B is a constant, $\alpha = 0.1 - 0.3$, R is the gas constant and activation enthalpies H^* range from 440 to 700 kJ/mole. Such a behavior confirms the broad distribution of relaxation times proposed in particular by Minster and Anderson (1981). In olivine, attenuation is known to depend on water content as well as on temperature (Jackson et al., 1992). In this case, equation (1) can be modified as:

$$Q^{-1}(\omega, T) = B'\omega^{-\alpha}(f_{H_{20}})^{\beta} exp(-\alpha H^*/RT) \tag{2}$$

where $f_{H_{20}}$ is fugacity of water and B' is a constant (see Karato and Jung, 1998). Equation (2) can be rewritten as,

$$Q^{-1}(\omega, T) = B\omega^{-\alpha} exp(-\alpha H^*/RT^*) \tag{3}$$

where T^* is the rheologically effective temperature (RET) defined by,

$$T = T * \xi \tag{4}$$

with

$$\xi = 1 - RT(logB'/B + \beta log f_{H_{20}})/(\alpha H^*) \tag{5}$$

where β is a parameter describing the effect of water on Q (see *Karato and Jung,* 1998). ξ is a weak function of T so in practice we can use a fixed T (background T) in calculating T*. At usual conditions in the Earth $\xi \sim 0.9 - 1.0$.

Seismic wave velocity at a given depth (i.e., pressure) can vary laterally due to the lateral variations in temperature and chemical composition. For a small effect of anelasticity, a general relation to express such a relation is (e.g.,*Minster and Anderson,* 1981):

$$V(\omega, T, C) = V_0(T, C)[1 - AQ^{-1}(\omega, T, C)] \tag{6}$$

where $V(\omega, T, C)$ is seismic wave velocity as a function of frequency, temperature, T, and C is chemical composition. The first term in this equation, $V_0(T, C)$, represents the anharmonic effect and the second term is the correction factor for anelastic effects, where $A = (1/2)cot(\pi\alpha/2)$ if the power-law behaviour of attenuation is assumed, as in equation (1).

Anharmonic effects can be determined by high frequency laboratory measurements and an extensive data set is available for a wide range of materials including oxides and most of silicate minerals (see e.g., *Anderson et al.,* 1992). The dependence of $V_0(T, C)$ on temperature and chemical composition has been well documented. ASnharmonic effects can also be calculated from first principles (e.g. Karki et al., 1999). The results are summarized as follows:

(1) To a good approximation, seismic wave velocity varies with temperature nearly linearly when only anharmonic effect is important (figure 2).

(2) The temperature derivatives corresponding to anharmonic effects decrease significantly with pressure.

(3) $V_0(T, C)$ depends on major element chemistry but is insensitive to minor element chemistry such as water content (figure 3).

The measurements of velocity dispersion and attenuation have been made so far on olivine (*Jackson et al.,* 1992), MgO (*Getting et al.,* 1997) and perovskite (*Webb et al.,* 1999) and support the relations (1) and (2). Although the data set for anelasticity is less comprehensive than that on anharmonicity, we can summarize the results as follows:

(1) The seismic wave attenuation (Q^{-1}) follows a power-law shown by equation (1) and changes non-linearly with temperature.

(2) Consequently, seismic wave velocity changes with temperature non-linearly when anelasticity is important (figure 2).

(3) For olivine, water is found to enhance anelasticity and hence reduce seismic wave velocity (*Jackson et al.,* 1992; *Karato,* 1995; *Karato and Jung,* 1998). Not much data are available for the role of major element chemistry such as Fe/(Fe+Mg) ratio, but based on the data on the dependence of diffusion or creep on Fe/(Fe+Mg), it can be concluded that a small change in major element chemistry has negligible effects on attenuation (figures 4,5).

Proposed Work: Solving directly for temperature using long period seismic waveform information

In this project, we propose to exploit the dependence on effective temperature and chemical composition of both velocity and attenuation, combined with our (imperfect) knowledge of mantle geotherms, in an attempt to solve directly for lateral variations in temperature and composition in the upper-mantle, by an appropriate parametrization of the model, and a waveform inversion approach, as developed by us over the last 5 years for elastic tomography (*Li and Romanowicz,* 1995, 1996; *Mégnin and Romanowicz,* 1999) as well as anelastic tomography (*Gung and Romanowicz,* 1999).

Combining phase and amplitude information in a single tomographic inversion procedure has the advantage of enabling us to exploit the stability of the phase part of the seismogram with the enhanced sensitivity of the amplitude to temperature. Such an approach has already been demonstrated in a somewhat different context, that of experimental studies of the internal structure of rock samples (Debski and Young, 1999), in which information on velocity and attenuation structure of the rock sample contained in waveforms is combined to obtain better insight into the rock microstructure.

We will proceed as follows. We will compute partial derivatives of the seismogram with respect to temperature and composition by first expressing each seismogram in terms of its dependence on elastic velocity and attenuation, using the normal mode summation approach as described for example, in *Li and Romanowicz* (1995, 1996). Partial derivatives with respect to velocity and attenuation, of the local frequency perturbations $\delta\omega$ (elastic) and $\delta\alpha$ (anelastic) can be readily obtained (e.g. *Li and Romanowicz,* 1996). Because amplitudes are strongly affected by focusing effects due to 3D elastic structure, as discussed previously, we will also include the contribution of focusing in the expression for the seismogram, as computed using higher order asymptotic theory, for which we have long ago derived normal mode-based expressions (*Romanowicz and Roult,* 1986; *Romanowicz,* 1987; *Romanowicz and*

Gung, in preparation). In a first stage, we will ignore the across-branch coupling terms corresponding to the NACT theory (Non Linear Asymptotic Coupling Theory) that are necessary to obtain accurate kernels for body waves (e.g. *Li and Romanowicz,* 1995), because we will be primarily interested in upper-mantle structure as derived from fundamental and higher-mode surface wave data, for which the PAVA theory has been shown to be adequate (e.g. *Mégnin and Romanowicz,* 1999). Adding NACT terms does not present any difficulty other than significantly larger computational time, and we will do that in the later stages of the project.

Let us now consider how velocity and attenuation can be parameterized in terms of temperature and chemical composition. From (2), it follows,

$$\delta logV(\omega, T, C) = \delta logV_0(T, C) + \delta logV'(\omega, T, C) \tag{7}$$

with

$$\delta logV'(\omega, T, C) = DQ^{-1}(\omega, T, C)\delta logQ^{-1}(\omega, T, C) \tag{8}$$

where a small attenuation ($Q^{-1} << 1$) is assumed and D is a constant. Thus the effects of anharmonicity (the first term) and the effects of anelasticity (the second term) can be clearly separated.

In inverting seismological data in terms of chemical and temperature variation, one needs to distinguish the effects of major element chemistry from those of water. Therefore there are basically three parameters (temperature, major element chemistry and water content) that can significantly affect velocity and attenuation of seismic waves. However, to facilitate the inversion, one can reduce them to two parameters as follows. First let us write the variation in velocity (due to anharmonic effects) and attenuation in terms of T, T^* and C (composition of major elements),

$$\delta logV_0(T, C) = E\delta T + F\delta C \tag{9}$$

and

$$\delta logQ^{-1} = E'\delta T^* + F'\delta C \tag{10}$$

with $F' \sim 0$ based on mineral physics showing that small changes in major element chemistry have little effect on rheology. Now, by noting that ξ is nearly unity ($\xi = 0.9 - 1.0$), equation (9) may be approximated by,

$$\delta logV_0(T, C) = E\delta T^* + F\delta C \tag{11}$$

(However, replacing T with T^* is important because even a small difference between T and T* can result in large differences in Q. But a small difference between T and T* does not result in significant difference in estimated C.) In this way, using both phase and amplitude of seismic waveforms, we can map out major chemistry and rheologically effective temperatures (RET) in the Earth's mantle. The key parameters here are E, F and E'. E and F have been well constrained by experimental and theoretical studies for most of mantle materials (see *Anderson et al.,* 1992; *Karato and Karki,* 2000). The parameter E' is determined by the activation enthalpy and background temperature. We use experimentally determined activation enthalpies where available (for olivine, MgO and perovskite). In regions where these data are not available, we use an empirical rule that the activation enthalpy is proportional to the melting temperature (see *Karato,* 1993). For a background (radially symmetric) temperature, we will use *Stacey*'s (1992) geotherm and adjust pre-exponential factors for Q to match radially symmetric model of Q (e.g. *Romanowicz and Durek,* 2000). The results of inversion do not strongly depend on the choice of background temperature. Such an inversion does not directly give temperature anomalies. However, $T*$ (RET) is directly related to lateral variation in rheology which is due both to the lateral variation in temperature and water content. Therefore such results have direct relevance to the lateral variation in rheology. Furthermore, in regions where water content is considered to be homogeneous, the map of effective temperature can directly be translated to a map of temperature. When major element chemistry is well constrained (this is the case for the oceanic upper mantle), then both temperature and water content may be estimated from such an inversion.

Effects of partial melting may complicate the issue. Under most of the upper mantle, large direct effects of partial melting are likely to be limited to the very vicinity of mid-ocean ridges or other volcanoes. Therefore in a spherical harmonic analysis up to degree of 12 or so, we can neglect these effects. A more important effect of partial melting is then the indirect effect through water depletion (*Karato and Jung,* 1998). This can affect velocity and attenuation in broader regions. However, such an effect is included when we invert the data for effective temperature, T*, and not for true temperature.

We will parametrize 3D temperature variations in terms of spherical harmonics laterally and either polynomials or layers vertically with the maximum order of the spherical harmonics development to be determined, by progressively inverting to higher orders (we expect to be able to achieve a resolution of on the order of degree 12, considering trade-offs between the resolution of velocity which now is possible to degrees 24 or higher, and the lower resolution of attenuation in standard inversion procedures).

In addition, because of uncertainties in the experimental results to date, in particular for the deeper parts of the upper mantle, we will solve for unknown variations in depth of the coefficients E, F and E' as defined above, using a low order polynomial expansion. The actual details of parametrization and choice of reference values for the radial variations of velocity, Q and temperature will be determined through iterative input from the mineral physics collaborators.

The dataset used will be the collection of long period SH waveforms assembled in the course of the construction of tomographic models SAW12D (*Li and Romanowicz,* 1996) and SAW24B16 (*Mégnin and Romanowicz,* 1999), complemented by additional data acquisition to fill gaps in the coverage, particularly in the southern hemisphere, assembled in the course of the waveform Q study of *Gung and Romanowicz* (1999). We will use similarly rigorous data selection criteria as in our previous Q studies, to minimize contamination by unwanted scattering effects that cannot be modelled using linear focusing theory. The mostly SH sensitive data set allows us to avoid, at this stage, the issue of upper-mantle anisotropy and its effects on the data. We will primarily use the the surface wave part of the data set (available down to a period of 80 s), complemented with wavepackets corresponding to the arrival of higher mode surface waves (available down to a period of 32 s). Depending on how the study evolves, we will progressively incorporate bodywave data, with the goal of ultimately increasing the depth range into the lower mantle.

Another issue that we will need to address are crustal corrections, for which we will combine the elastic results of *Mooney et al.* (1998) and anelastic compilations of Mitchell and collaborators (*Mitchell,* 1995).

Work Plan

The first year will be devoted to exploring the optimal parametrization from the mineral physics point of view, namely the dependence of seismic wave velocity on temperature, major element chemistry and water, as well as modifying the existing seismic waveform inversion codes accordingly and performing tests on lateral and depth resolution of the various parameters. The seismic coding and inversion will be performed by graduate student Y.C. Gung, who now has 2 years experience with the U.C. Berkeley codes.

We will follow the theoretical scheme outlined above to quantify the effects of temperature, major element chemistry and water on seismic velocity and attenuation (to constrain constants E, E' and F as a function of depth). In evaluating the effect of temperature, we will distinguish the effects of anharmonicity and of anelasticity. A large number of experimental data are available on the effects of anharmonicity, but the cross derivatives (with respect to T and P) are not well constrained. Karato and Karki (a post-doc) will investigate the anharmonicity term by a theoretical method. We will calculate the cross derivatives for olivine, puroxenes, wasdsleyite and rigwoodite using the first principle technique. Karki has a strong background in first principles calculation of elasticity of minerals (*Karki et al.,* 1999). These cross derivatives contribute significantly to the depth variation in temperature sensitivity of seismic wave velocities. The anelastic effects also contribute equally to the temperature sensitivity of seismic wave velocity (*Karato,* 1993). This term is also depth dependent. We will use various models to estimate the pressure dependence of activation enthalpy, namely the activation volume including the homologous temperature scaling (e.g., *Weertman,* 1970) or the strain energy model (*Keyes,* 1963). This estimate has some uncertainties which however have relatively small effects on calculated temperatures. The effects of major element chemistry will be calculated using the published data source (e.g., *Bass,* 1995). The effects of major element chemistry on anelasticity is difficult to estimate. We will use the known dependence of diffusion or creep on major element chemistry to infer the dependence of anelasticity on major element chemistry. This inference has large uncertainties, but the effects of major element chemistry (e.g. Fe/(Fe+Mg) ratio) are expected to be small. The effects of water on anelasticity are large but not very well constrained (*Karato and Jung,* 1998). We will formulate water effects using available data on attenuation (e.g.,*Jackson et al.,* 1992) and on creep and grain-boundary mobility. In particular, quantitative data on the effects of water on creep and grain-boundary mobility are now available (e.g., *Mei and Kohlstedt,* 2000) which provide useful constraints on the effects of water on attenuation.

In the second year, we will finalize the model of global variations in temperature and chemical composition in the upper mantle and proceed with its geodynamical interpretation, bringing in correlations with other observations, such as provided by geochemistry, and further insights from mineral physics and tectonics, as well as seismology.

Contribution to human resources This work will contribute directly to the training of one graduate student (Y.C. Gung) and one post-doc (B. Karki) as well as indirectly, through research group meetings, to the training of 6 graduate students in seismology at U.C. Berkeley and 2 graduate students in mineral physics at Univ. of Minnesota.