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Impact of phase transitions on P wave velocities

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ABSTRACT

In regions where a high pressure phase is in equilibrium with a low pressure phase, the bulk modulus defined by the *P*–*V* relationship is greatly reduced. Here we evaluate the effect of such transitions on the P wave velocity. A model, where cation diffusion is the rate limiting factor, is used to project laboratory data to the conditions of a seismic wave propagating in the two-phase region. We demonstrate that for the minimum expected effect there is a significant reduction of the seismic velocity, as large as 10% over a narrow depth range.

1. Introduction

Acoustic velocities serve as the primary window that we have to the Earth's interior. Seismic velocities are the best resolved and most accurately defined property of the materials that makes up the deep Earth that is available to us. It brings information about chemical composition, temperature, flow fields, and crystal structure. It's remarkable power, in part, lies in the robust character of this property. Sound velocities are generally the same at GHz frequencies as they are at mHz frequencies. This has meant that laboratory measurements of acoustic velocity with wavelengths comparable to that of visible light (500 nm), such as with Brillouin spectroscopy, provides constraints on velocities of surface waves with wavelengths of a few hundred km. The breakdown of this relationship occurs if there is a process whose time scale is between that of the laboratory and that of the field that can relax the strain by a non-elastic response (Anderson, 1989; Anderson and Given, 1982; Brennan and Stacey, 1977). Typically, dislocation motion, grain boundary sliding, or melt flow are the types of processes that are considered in this manner (Gribb and Cooper, 1998; Jackson, 2007; Jackson et al., 1992) and these affect mainly the shear modulus. However, first order phase transitions can affect both the bulk modulus and the shear modulus (Anderson, 1989; Jackson, 2007; Li and Weidner, 2008; Ricard et al., 2009; Tamisiea and Wahr, 2002; Vaisnys, 1968).

Seismic waves such as P waves and S waves travel through the vibration of the particles with an associated stress and strain. The velocity is controlled by the ratio of the stress to the strain. In most circumstances, this strain is controlled by the forces between atoms. If the stress drives a phase transition, then the resulting strain is increased, thus reducing the sound velocity. Since the stress of an elastic wave is so small, we expect effects of phase transitions only in regions where both the high pressure phase and the low pressure phase coexist. Then, the stress wave simply changes the ratio of abundance of the two phases, but in the process, a volume change occurs. It is common for the high and low pressure phases to coexist over a pressure interval as one chemical component is partitioned between the two phases. For the olivine to wadsleyite transition, the iron to magnesium ratio of the system is responsible for creating this two-phase loop (see Fig. 1). Within a peridotitic mantle, several phase transformations occur with depth. Olivine transforms to wadsleyite, then to ringwoodite, then to perovskite plus magnesiowustite, then to postperovskite plus magnesiowustite. The pyroxene component transforms to garnet, then to perovskite, then to postperovskite. Iron bearing phases experience a high spin to low spin transition. Partial melting may

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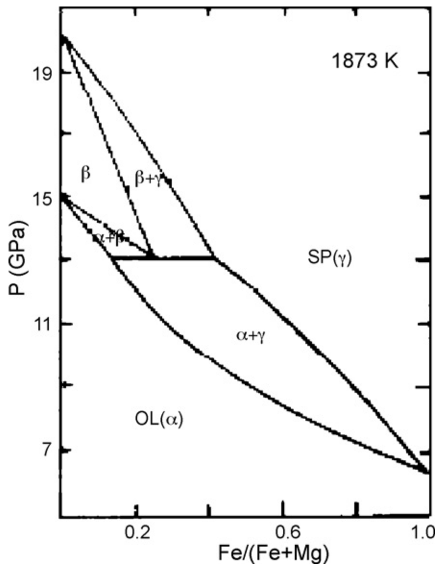

Fig. 1. Phase diagram of olivine at 1873 K. The region that undergoes transformation must change composition by crossing the two-phase loop. P_{tran} is given by the vertical height of the two-phase loop.

occur. All of these transitions involve a volume change and occur over a depth range, e.g. the width of the discontinuities at 410 km, 520 km, and 660 km, etc.

Previous studies (Anderson, 1989; Jackson, 2007; Tamisiea and Wahr, 2002) have reported the possible impact of the phase transitions on velocities, but have not defined the magnitude of the effect (Li and Weidner, 2008) demonstrated the effect of total relaxation of the phase transitions. Here we explore the relevant description of these transitions within a periodotitic mantle for P waves with an emphasis on the likely impact of these transitions on mantle velocities. We conclude that only an approach to equilibrium is likely, but there should be a significant signature on the mantle seismic velocity.

2. Model

That phase transformations can cause velocity decreases is well established (Anderson, 1989; Jackson, 2007; Li and Weidner, 2008; Vaisnys, 1968). The process of an acoustic wave driving a phase transformation fits the criterion of an anelastic solid. The material is completely characterized by defining a relaxed modulus, an unrelaxed modulus, and the characteristic time. This may be a single time or a distribution of time (Anderson, 1989).

The relaxed bulk modulus is the ratio of the pressure change to the volume strain, where volume strain includes elastic compression and the strain impact of the phase transition that results from the pressure change or:

$$K_{relaxed} = \rho \frac{\partial P}{\partial \rho} \tag{1}$$

where the density vs pressure curve includes the effects of phase transformation as well as compression. For the models discussed below, we first construct a density vs pressure model that reflects the relevant phase transformations and elastic properties. The relaxed modulus is obtained by differentiating this curve. For visualization purposes, one can approximate this relation as follows:

$$-\frac{\delta V}{V} = -\frac{\delta P}{P_{tran}}\left(\frac{\Delta V}{V}\right)_{tran} + \frac{\delta P}{K_{elas}} = \frac{\delta P}{K_{relaxed}} \tag{2}$$

where δV and δP are the associated volume change and pressure change, P_{tran} is the width of the two-phase region, K_{elas} is the elastic bulk modulus, ΔV is the volume change of the phase transition, and $K_{relaxed}$ is the relaxed bulk modulus. In this equation, we use the approximation that the fraction of material that undergoes the transition is $\delta P/P_{tran}$. The unrelaxed elastic modulus is simply the aggregate bulk modulus, K_{elas}. In Fig. 1 we identify P_{tran} for the olivine system as the pressure–width of the two-phase loop.

Our picture of the phase transition is one where the high pressure phase, with one composition, is in contact with the equilibrium composition of the low pressure phase. Then the change in phase proportions is accomplished by movement of the boundary between the two phases. This yields the distance that the phase boundary moves as a characteristic length. The characteristic time is related to a characteristic length by either a velocity if the process is a rate process:

$$\tau = \frac{x}{\nu} \tag{3}$$

or through a diffusion equation if the process is diffusion controlled:

$$\tau = \frac{x^2}{D} \tag{4}$$

where τ is the characteristic time, x is the characteristic length, ν is the velocity of the rate process, and D is the appropriate diffusion coefficient. Both of these processes are required to move the boundary. Since the composition of the low pressure phase is different than that of the high pressure phase as is evident in the phase diagram in Fig. 1, then diffusion must occur to change the composition of the region that transformed. The time scale of this process is controlled by the appropriate diffusion coefficients. Furthermore, since the crystal structure of the two phases is different, a reconstruction front needs to move through this region. This process is often described by a velocity of the form:

$$\nu = AT\ \exp\left\{-\frac{\Delta H + PV^*}{RT}\right\}\left(1 - \exp\left\{\frac{-\Delta G}{RT}\right\}\right) \tag{5}$$

where A is a constant, T is temperature, ΔH is the activation enthalpy, P is pressure, V^* is the activation volume, and ΔG is the excess Gibbs free energy arising from the stress in the acoustic wave (Kubo et al., 2004; Turnbull, 1956). Since this latter quantity is quite small, we can replace the term in parenthesis by $\Delta G/RT$ or by $\Delta V\delta P/RT$ where ΔV is the volume change of the phase transition and δP is the excess pressure associated with the stress wave. Since all other values remain constant as the wave moves through the system, we have:

$$\nu = B\delta P \tag{6}$$

or simply, transformation rate, and hence velocity, is proportional to pressure perturbation.

The geometry of a model where growth is the dominant process is illustrated in Fig. 2. A sphere of one phase grows by adding a small rim (Jackson, 2007; Li and Weidner, 2007; Ricard et al., 2009). In this case nucleation is not required. This system yields a characteristic length, x, which is the width of the rim that is added to a grain of dimension, d. If the width of the rim is limited by the phase diagram it is given by (Jackson, 2007; Li and Weidner, 2008):

$$x \sim \left(\frac{d}{3}\right)\frac{\delta P}{P_{tran}} \tag{7}$$

Ricard et al. (2009) calculates the characteristic length based on the assumption of a spherical inclusion coupled with the elastic support of the matrix. In this case, the volume change of the phase transformation will locally reduce the stress and stop further transformation if supported by the strength of the matrix. They find:

$$x \sim \left(\frac{d}{3}\right)\frac{\delta P}{3K_{elas}} \tag{8}$$