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A new method for calculating seismic velocities in rocks containing strongly dimensionally anisotropic mineral grains and its application to antigorite-bearing serpentinite mylonites

Tohru Watanabe [a,*], Yuhto Shirasugi [a], Katsuyoshi Michibayashi [b]

[a] Department of Earth Sciences, Graduate School of Science and Engineering, University of Toyama, 3190 Gofuku, Toyama 930-8555, Japan
[b] Institute of Geosciences, Shizuoka University, 836 Ohya, Suruga-ku, Shizuoka 422-8529, Japan

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ABSTRACT

Seismic velocity is one of the most important sources of information about the Earth's interior. For its proper interpretation, we must have a thorough understanding of the dependence of seismic velocity on microstructural elements, including the modal composition, the crystal preferred orientation (CPO), the grain shape, the spatial distribution of mineral phases, etc. The conventional Voigt, Reuss and Hill averaging schemes take into account only the modal composition and the CPO. The information about the Earth's interior is thus poorly constrained. For a better interpretation, it is critical to have a calculation method which accounts for the grain shape and the spatial distribution of mineral phases, etc. We propose a calculation method which accounts for the grain shape of strongly dimensionally anisotropic minerals like micas and serpentines. Our method can be applied to a distributed geometrical orientation of mineral grains. Comparison was made between calculated and measured velocities in three antigorite–serpentinite mylonites. Judging from the root mean square relative error, our method provides velocities closer to measured values than the Voigt, Reuss and Hill averaging schemes. The input of the grain shape considerably improves the prediction of seismic properties. However, large discrepancies (>0.1 km/s) between measured and calculated velocities can be seen in some directions. The discrepancies might come from microstructural elements which were not considered in the calculation (layer structures and cracks).

1. Introduction

Seismic velocity is one of the most important sources of information about the composition, structure and dynamics of the Earth's interior. The seismic velocity of a rock is governed by its effective elastic constants and bulk density. The bulk density is simply the volumetric average of densities of constituent minerals. On the other hand, the effective elastic constants depend on single-crystal elastic constants of constituent minerals and various microstructural elements, including the modal composition, the crystal preferred orientation (CPO), the grain shape, the spatial distribution of mineral phases, the properties of grain boundaries, and the presence of porosity and fluids (e.g., Mainprice and Humbert, 1994; Mainprice et al., 2000; Wendt et al., 2003; Valcke et al., 2006; Naus-Thijssen et al., 2011). For simplicity, this paper will focus on polycrystalline materials without porosity or fluids. Single-crystal elastic constants have been well studied for most rock-forming minerals via the resonant ultrasound spectroscopy (e.g., Isaak and Ohno, 2003) and the Brillouin-spectroscopy (e.g., Murakami et al., 2012). It is necessary to have a thorough understanding of the dependence of effective elastic constants on microstructural elements.

Most studies so far have calculated effective elastic constants considering only the modal composition and the CPO. The most simple calculation methods are the Voigt (1928) and Reuss (1929) averaging schemes. The Voigt average gives an upper bound and the Reuss average a lower bound to elastic stiffness (Hill, 1952). A physical estimate of the elastic stiffness should lie between these bounds. Based on measured elastic constants of polycrystalline metals, Hill (1952) suggested that the arithmetic and geometric means of the Voigt and Reuss averages are good approximations to the actual elastic constants. The arithmetic mean is known as the Hill or Voigt–Reuss–Hill (VRH) average. For its simplicity, the Hill average has been employed by a lot of works to study the influence of the modal composition (e.g., Tatham et al., 2008; Lloyd et al., 2009, 2011; Ward et al., 2012) and the CPO (e.g., Lloyd et al., 2009, 2011) on seismic properties of rocks.

It should be noted that the Hill average has no physical justification (Watt et al., 1976). It is just an arithmetic mean of the Voigt and Reuss averages. For a two-component isotropic

* Corresponding author. Tel.: +81 76 445 6650; fax: +81 76 445 6549.
E-mail address: twatnabe@sci.u-toyama.ac.jp (T. Watanabe).

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composite material, Watt et al. (1976) showed that the difference between the Voigt and Reuss averages increases with increasing differences in elastic moduli between two components. Later, Mainprice and Humbert (1994) studied the influence of the elastic anisotropy of a mineral on the difference between the Voigt and Reuss averages for a randomly oriented monomineralic polycrystalline aggregate. The difference between two averages increases with increasing anisotropy of constituent minerals. When constituent minerals have similar elastic moduli and weak anisotropy, the difference between the Voigt and Reuss averages is relatively small. The Hill average can provide a good prediction of elastic properties. When strongly anisotropic minerals like micas or serpentines are contained, the Hill average is an estimate with large uncertainty (Mainprice and Humbert, 1994; Wenk et al., 2012). The difference between the Voigt and Reuss averages shows that other microstructural elements such as grain shape and spatial distribution of grains have a noticeable influence on effective elastic constants (e.g., Bunge et al., 2000), especially in rocks containing strongly anisotropic minerals.

Comparisons between measured and calculated velocities have suggested the importance of the grain shape fabric and the spatial distribution of grains in controlling elastic properties of rocks (Burlini and Kunze, 2000; Kern et al., 2008; Watanabe et al., 2011). Burlini and Kunze (2000) and Kern et al. (2008) suggested that the strong shape preferred orientation (SPO) significantly contributed to the observed anisotropy. Moreover, Burlini and Kunze (2000) suggested the preferred alignment of accessory mineral phases along grain boundaries as a source of anisotropy. Watanabe et al. (2011) suggested that the closeness of velocities in serpentinite mylonites to Reuss averages was attributed to the platy grain shape of antigorite and the well-developed shape fabric. For a further understanding of elastic properties of rocks, it is critical to have a calculation method which accounts for the grain shape and the spatial distribution of grains.

We have formulated a calculation method which accounts for the grain shape. In this paper, we present this calculation method and show its application to antigorite-bearing serpentinites. Several calculation methods have been already proposed to take into account the influence of the grain shape (e.g., Nishizawa and Yoshino, 2001; Wendt et al., 2003; Naus-Thijssen et al., 2011; Wenk et al., 2012; Morales et al., 2013). Nishizawa and Yoshino (2001) treated a mica grain as an oblate spheroidal inclusion to calculate effective elastic constants of mica schists. Their method was limited to the case where oblate spheroidal inclusions are completely aligned. We extend their method to a distributed geometrical orientation of grains. Compared with other methods, this method is relatively simple and easy to understand. We first briefly review previous works on effective elastic constants of composite materials, and then describe the method of Nishizawa and Yoshino (2001) and its extension to a distributed geometrical orientation of grains. Our method is applied to antigorite-bearing serpentinites, and calculated and measured velocities are compared. Though the input of the grain shape improves the agreement between measured and calculated values, there are still discrepancies between them. The causes of discrepancies are discussed.

2. Calculation of effective elastic constants

2.1. Previous works

We first show the macroscopic constitutive equation of a composite material. Let us consider a composite material which is microscopically heterogeneous but macroscopically homogeneous. It contains many regions, which are compositionally and structurally similar. Effective elastic constants, $\boldsymbol{C}^*$ relate the average stress, $\langle \boldsymbol{\sigma} \rangle$ to the average strain, $\langle \boldsymbol{\varepsilon} \rangle$ in the composite material as

$$\langle \boldsymbol{\sigma} \rangle = \boldsymbol{C}^* \langle \boldsymbol{\varepsilon} \rangle.$$

The average stress and strain are defined by

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{V} \int \boldsymbol{\sigma}(\boldsymbol{x})\, dv$$

and

$$\langle \boldsymbol{\varepsilon} \rangle = \frac{1}{V} \int \boldsymbol{\varepsilon}(\boldsymbol{x})\, dv,$$

where V is the volume of a considered region and dv the volume element at point $\boldsymbol{x}$ (Watt et al., 1976). The local stress, $\boldsymbol{\sigma}(\boldsymbol{x})$ and strain, $\boldsymbol{\varepsilon}(\boldsymbol{x})$ are related by Hooke's law as

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{x})\boldsymbol{\varepsilon}(\boldsymbol{x}),$$

where $\boldsymbol{C}(\boldsymbol{x})$ is the elastic stiffness tensor at point $\boldsymbol{x}$. For simplicity, we focus on polycrystalline materials without porosity or fluids. Since the structural details of a composite material are in general never known, it is impossible to calculate exact effective elastic constants. A number of methods have been devised for evaluating effective elastic constants. They are classified into three groups by the used microstructural information (Mainprice et al., 2000). Group 1 uses the modal composition and the CPO, Group 2 the modal composition, the CPO and the grain shape, and Group 3 the modal composition, the CPO, the grain shape, and the spatial distribution of mineral grains.

Group 1

The simplest and best known methods of this group are the Voigt (1928) and Reuss (1929) averaging schemes. The Voigt average is obtained by assuming a uniform strain field, while the Reuss average assumes a uniform stress field. The Voigt average gives an upper bound, and the Reuss average a lower bound to elastic stiffness (Hill, 1952). The arithmetic mean of the Voigt and Reuss averages is known as the Hill or Voigt–Reuss–Hill (VRH) average. The Hill average has been used as a useful estimate, although it has no physical justification.

The geometric mean (Morawiec, 1989; Matthies and Humbert, 1993) imposes the constraint that the ensemble average of elastic stiffness $\langle \boldsymbol{C} \rangle$ should be equal to the inverse of the ensemble average of elastic compliances $\langle \boldsymbol{S} \rangle^{-1}$. This seems to be a strong physical basis. However, the geometric mean gives results very similar to the Hill average (Mainprice and Humbert, 1994). Thus, it might be just another type of mean estimate with no additional significance (Mainprice et al., 2000).

Group 2

This group uses the information about the grain shape to take into account the mechanical interaction between mineral grains. Adding a mineral grain into a homogeneous matrix changes the elastic strain energy of the matrix, which can be evaluated by using Eshelby's (1957) solution for the elastic field of an ellipsoidal inclusion. The effective elastic constants of a new composite material can be derived by differentiating the elastic strain energy (Eshelby, 1957). The self-consistent schemes (SCS) were proposed to take into account the interactions between elastic elements (Hill, 1965; Budiansky, 1965). A mineral grain is embedded in a homogeneous matrix with the effective elastic constants to be determined. Later, Bruner (1976) and Henvey and Pomphrey (1982) pointed out that the SCS progressively overestimates the interaction between mineral grains with their increasing concentration. They proposed an alternative differential effective medium (DEM) method in which the concentration of inclusions is increased by small steps with a re-evaluation of effective elastic constants of the aggregate at each increment.