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Impact of grain shape on seismic attenuation and phase velocity in cubic polycrystalline materials

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HIGHLIGHTS

- We investigate the propagation properties of anisometric polycrystalline aggregates.
- Attenuation and phase velocity are computed using a spectral function approach.
- Attenuation and phase velocity vary with the grain shape/size and the frequency.
- q-*SV* and q-*SH* attenuations differ in the Rayleigh-to-Stochastic transition regime.
- q-*SV* and q-*SH* phase velocities differ from the Rayleigh to the Stochastic regime.

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ABSTRACT

Attenuation and phase velocity of seismic waves propagating in cubic polycrystalline aggregates with elongated grains are computed from the Rayleigh (low-frequency) to the geometrical optics (high-frequency) regime using a spectral function approach. In this study, we consider the case of perfectly aligned ellipsoidal grains with randomly oriented crystallographic axes. Such anisometric medium exhibits transverse isotropy. The frequency dependence of both phase velocity and scattering attenuation for quasi-compressional (q-*P*), quasi-shear vertical (q-*SV*) and quasi-shear horizontal (q-*SH*) waves are examined in detail. The attenuation depends on the effective volume of the grain in the Rayleigh regime, on the grain dimension in the direction of propagation in the stochastic regime, and is inversely proportional to the grain size in the direction of propagation in the geometrical optics regime. The phase velocity exhibits a much more complex pattern depending on the grain shape and frequency. In particular, the fast/slow direction of propagation is not systematically aligned with the direction of low/high attenuation. The anisotropy in velocity typically varies from 1% in the Rayleigh regime to a few percents at the transition from the stochastic to the geometrical optics regime. Even for a highly anisotropic cubic iron crystals, q-*SV* and q-*SH* attenuations differ by at most 12% in the Rayleigh-to-stochastic transition regime but are equal in other frequency ranges. The q-*SV* and q-*SH* phase velocities, from the Rayleigh to the stochastic regime, differ by at most 1%. Anisotropy induced by geometrical effects should therefore be detectable in laboratory or seismological data.

1. Introduction

Propagation and scattering of elastic waves in heterogeneous media is an important topic of interest in seismology, non-destructive testing and materials characterization [1–3]. In particular, scattering in polycrystalline materials has

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received considerable attention [4–11]. Experimental studies demonstrate that microstructural properties of polycrystalline aggregates, i.e. crystal anisotropy, grain size and elongation, preferential orientation of crystallites and grains, strongly affect the scattering attenuation and the phase velocity of elastic waves which propagate through such media. Robust and quantitative theoretical models are thus necessary to characterize microstructural parameters and textures from ultrasonic or seismic measurements.

The theory of multiple scattering in random media developed in the sixties by Karal and Keller [12] has been applied to the propagation of elastic waves in untextured polycrystals with equiaxed grains by Stanke and Kino [5]. They derived algebraic equations governing the effective wave number and solved these equations numerically to investigate the frequency dependence of the phase velocity and attenuation for longitudinal and transverse waves from the Rayleigh to the geometrical optics regimes. Weaver [8] obtained a general solution for attenuation and diffusivity of ultrasound in untextured cubic polycrystals using the Dyson and Bethe–Salpeter equations within the limits of the first-order smoothing approximation [13]. He also used an additional approximation (Born approximation) which restricts the results to frequencies below the geometrical optics regime. This approach has been subsequently extended to other crystal symmetries (hexagonal or orthorhombic) [14–17] or to more complex textures [11,18].

In many materials, we observe significant grain deformation and elongation resulting from plastic deformation or directional solidification induced by industrial or natural processes [19–22]. Ahmed and Thompson [19] extended Stanke and Kino's model to cubic polycrystalline aggregates with perfectly aligned [001] crystallographic axes and grains elongated in the same direction. Wave propagation in such an aggregate exhibits angular dependence with respect to the preferred direction. For this specific texture, Ahmed and Thompson [19] observed that scattering attenuation for both longitudinal and horizontally polarized shear waves increases with the elongation of the grain. These models have been subsequently generalized for arbitrary crystallite symmetry and macroscopic texture [17,23]. For perfectly aligned elongated grains with randomly oriented crystallographic axes, the medium is still characterized by a macroscopic anisotropy and is referred to as anisometric [24]. For such aggregates, Ahmed et al. [25] argue that longitudinal attenuation and phase velocity are hardly affected by the grain elongation from the Rayleigh regime to the stochastic regime. More recent studies have mainly focused on the impact of grain shape on the attenuation only. Yang et al. [26] investigated more deeply the impact of grain shape on longitudinal and transverse attenuations in cubic polycrystalline media with perfectly aligned ellipsoidal grains based on Weaver's approach. They obtained explicit expressions for the attenuations in the Rayleigh and stochastic regime. They demonstrated that attenuation in the Rayleigh limit is independent of the grain shape and is controlled by the grain volume, while it varies linearly with the dimension of the grain in the direction of propagation in the stochastic regime. Later, Yang et al. [27] have extended the theory to hexagonal ellipsoidal grains and showed that attenuations are inversely proportional to the grain dimension in the direction of propagation in the geometrical optics regime. Recently, Rokhlin et al. [28] have explored the effect of the grain shape on the attenuation of longitudinal and transverse waves from the Rayleigh to the geometrical optics regime using a new scattering model based on a far-field approximation of the reference Green's function and simplifications of the mass-operator in addition to the first-smoothing approximation. Their results are in agreements with previous ones obtained by Yang and co-authors.

To date, all theoretical studies have neglected the possible splitting of S waves by anisometric heterogeneities in polycrystals. In this work, we propose to further develop Yang's model by discussing in detail the impact of grain shape on phase velocity, and by distinguishing explicitly between quasi-shear vertical (q-SV) and quasi-shear horizontal (q-SH) waves. As S-waves splitting is commonly observed in seismology, our work bears direct relevance to the structural interpretation of anisotropy in the Earth. To carry out this work, we adopt a spectral function approach [16] and compute numerically the attenuation and the phase velocity of quasi-compressional (q-P), quasi-shear vertical (q-SV) and quasi-shear horizontal (q-SH) waves from the Rayleigh to the geometrical optics regimes. In Section 2, we develop the analytical expressions of the mass operator for cubic polycrystalline aggregate in anisometric media with transverse isotropy. In Section 3, we present the numerical results and discuss the impact of grain shape on both attenuation and phase velocity for all wave types.

2. Dyson equation in anisometric media

2.1. Description of an anisometric medium

In this paper we consider a polycrystalline aggregate whose grains look like disks or cigars (Fig. 1). We assume that the grains are preferentially aligned but that the orientation of crystallographic axes varies from grain to grain (no crystallographic texture). The ellipsoidal shape of the grain is represented by a spatial correlation function of the form:

$$\eta(x, y, z) = \exp\left(-\sqrt{\frac{x^2}{a_x^2} + \frac{y^2}{a_y^2} + \frac{z^2}{a_z^2}}\right) \tag{1}$$

where (a_x, a_y, a_z) are the ellipsoid radii in the global cartesian (x, y, z) coordinate system [29,26,27]. It is a generalization of the exponential correlation function for equiaxed grains [5,8] which properly describes the variable shapes and linear