

Elastic moduli of anisotropic clay

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ABSTRACT

Clay minerals are important components in shales, controlling their elastic properties and anisotropy. The elasticity of crystalline clay minerals differs significantly from that of clay in situ because of the ability of clay particles to bind water. In the majority of published works, only isotropic moduli for in situ clays are reported. However, anisotropy is inherent in the clay elasticity. We develop an inversion technique for determination of the stiffness tensor of in situ clay from the shale's stiffness tensor. As an example, we obtain the stiffness tensor of a "water-clay" composite from the data on the water-saturated Greenhorn shale sample, whose clay composition consists of almost equal amounts of illite and smectite and comparable amounts of kaolinite and chlorite. The stiffness tensor of the water-clay composite is found for the Greenhorn shale with step-by-step inversion based upon an effective medium theory. The inversion uses

a nonlinear optimization technique with bounds imposed on the estimated parameters. In the inversion, we apply different approaches of the effective medium theory using a published method referred to here as the generalized singular approximation (GSA). The GSA method makes it possible to take into account the microstructure of shales. The resulting elasticity constants of the anisotropic (transversely isotropic) in situ clay composite are $C_{11} = 23.7$, $C_{33} = 8.5$, $C_{44} = 0.8$, $C_{66} = 5.7$, and $C_{13} = 3.1$ (in GPa); and the density equals 2.17 g/cm^3 . The Thomsen parameters for the clay composite are $\epsilon = 0.89$, $\gamma = 3.10$, and $\delta = -0.34$. The elasticity constants found for this clay composite can be used in the theoretical analysis of shales that have a similar composition of clay but with different mineral compositions. The inversion technique developed can be used for general shale water-clay composites when the mineral composition and orientation of the clay platelets are known.

INTRODUCTION

Clay minerals (phyllosilicate minerals are meant, not grain size) are one of the major components of sedimentary rocks including hydrocarbon reservoirs. The presence of clay minerals in shales governs their elastic properties and anisotropy. Shales constitute over 75% of the elastic fill of sedimentary basins (Jones and Wang, 1981). Consequently, knowledge of clay elastic properties is significant for the interpretation of seismic and sonic measurements.

Monocrystals of clay minerals are very thin platelets exhibiting considerable anisotropy of elastic properties. The stiffness tensor of clay minerals is of monoclinic symmetry (Vaughan and Guggenheim, 1986; Sato et al., 2005). Nonetheless, some authors point out that the elasticity symmetry of clays is approximately hexagonal with the principal c -axis of a crystal being the symmetry axis. This approximation is a good one because effects of the lower symmetry

are comparable to uncertainties in composition and structure for clays in shales (Alexandrov and Ryzhova, 1961; Katahara, 1996).

The elastic wave velocities in clay monocrystals are rather high. For example, the compressional wave velocities in the principal directions of a muscovite crystal, which is a structural and compositional analog of illite (Tosaya, 1982), are 7.93, 7.84, and 4.50 km/s. These values are calculated from the stiffness tensor of muscovite found by Vaughan and Guggenheim (1986).

Clay mass in rocks is made up of blocks consisting of subparallel, very thin (a few nanometers) phyllosilicate monocrystals (sheets) with a separation of 1 to 3 nm (Aylmore and Quirk, 1960). When water-saturated, their surfaces are separated by sheets of bound water, and much of the water may be bound to the surfaces due to the small distance between the clay platelets. Sayers (2005) mentioned that the bound water may form an ordered structure with a nonzero shear modulus. Sun et al. (1986) pointed out that water in smectite is less

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compressible than bulk water, and the type of exchange cations may control its properties (Guven, 1992). Thus, in shales, clay can be considered as an anisotropic clay-water composite. The elasticity moduli of the composite are lowered by the presence of the water within the clay mass.

The amount of incorporated water is different for different clays. Thus, the smectite sheets are of 1 nm thickness, between which there are one or more monolayers of water. The thickness of illite sheets is approximately 7 nm. According to Katahara (1996), the volume of water incorporated by smectite is five times greater than the water volume in an illite clay mass. Thereby, the properties of a smectite clay mass are mostly governed by the incorporated water, and as a result, a dramatic change (decrease) in elastic properties can be expected compared to those of illite and other clays.

The elastic properties of clays have been estimated by many authors. Katahara (1996) present velocities for isotropic polycrystals of illite, chlorite, and kaolinite calculated with the Voigt-Reuss-Hill (VRH) averaging (Hill, 1952) from the respective stiffness tensors given by Alexandrov and Ryzhova (1961). These velocities are rather high: $V_p = 5.82$ km/s and $V_s = 3.37$ km/s for illite; $V_p = 5.93$ km/s and $V_s = 3.35$ km/s for chlorite; and $V_p = 6.23$ km/s and $V_s = 3.55$ km/s for kaolinite. When calculating the velocities for illite, the stiffness tensor of muscovite was used because of the structural and compositional similarity of these minerals.

Several authors estimated the isotropic velocities in clays from empirical dependencies of velocities on porosity and shale content that were derived from logging data or laboratory measurements. In this approach, the velocities are determined as an extrapolation of the dependences to pure clay. Using logging data for sandstones of the Frio formation, Castagna et al. (1985) extrapolate the velocities for clay as $V_p = 3.60$ km/s and $V_s = 1.85$ km/s, which is a montmorillonite-illite mixture (Li, 2006). These velocities are close to the values derived by Tosaya (1982) from the similar dependences obtained for the laboratory data of a mixed clay: $V_p = 3.40$ km/s and $V_s = 1.60$ km/s. Similar velocities, $V_p = 3.41$ km/s and $V_s = 1.63$ km/s, for mixed clays were extrapolated by Han et al. (1986) from laboratory data. The logging-based extrapolation for illite is $V_p = 4.2$ km/s and $V_s = 2.5$ km/s (Eastwood and Castagna, 1986). These velocities are significantly lower than the velocities found by Katahara (1996) with the VRH averaging.

The isotropic properties of clay are also found from measurements on cold-pressed clay aggregates, clay powder, and water-clay suspension (Vanorio et al., 2003) or derived theoretically from elastic wave velocities measured on artificial samples made from clay particles and epoxy resin (Wang, 2002). Vanorio et al. (2003) give the isotropic properties of smectite as $V_p = 2.3$ km/s, $V_s = 1.3$ km/s, and the density equal to 2.29 g/cm³. The kaolinite properties found in this work are $V_p = 2.78$ km/s, $V_s = 1.52$ km/s, and 2.59 g/cm³ as the density. The latter values are in agreement with the elastic properties found by Prasad et al. (2002) using Atomic Force Acoustic Microscopy (AFAM). The elastic wave velocities of various clays theoretically inverted from measurements on clay-epoxy artificial samples are higher (Wang et al., 2001). For kaolinite, they obtained $V_p = 5.5$ km/s, $V_s = 3.01$ km/s, and the density equal to 2.44 g/cm³. Their values for smectite are $V_p = 2.78$ km/s, $V_s = 1.70$ km/s, and density equals 2.40 g/cm³. For illite, $V_p = 5.89$ km/s, $V_s = 3.06$ km/s, and density equals 2.71 g/cm³; and for an illite-smectite mixture (60%:40%) $V_p = 4.90$ km/s, $V_s = 2.67$ km/s, and the density equals 2.55 g/cm³.

The lowest velocities of clays are given by Woeber et al. (1963), who obtained $V_p = 1.44$ km/s, $V_s = 0.93$ km/s, and density equal to 1.58 g/cm³ for kaolin. However, it is not clear if these velocities were measured for the mineral kaolinite or for a porous rock.

Note that in most of the works mentioned, the velocities are measured in only one direction. However, the results are generalized to the whole sample as if it were isotropic. Only Prasad et al. (2002) pointed out that their results should be related to the C_{11} direction.

GREENHORN SHALE STUDIES

Sayers (2005) was the first to report on the anisotropic elastic properties of a water-clay composite. He inverted the stiffness tensor from the stiffness tensor of the Greenhorn shale sample recovered from a depth of 5000 ft (Jones and Wang, 1981; Hornby et al., 1994), whose composition is quartz 53%, clay 27%, feldspar 11%, and pyrite 9%. The clay consists of illite (36%), smectite (34%), kaolinite (17%), and chlorite (13%). The components of the stiffness tensor of the Greenhorn shale sample were found by Jones and Wang (1981, p. 293) from the velocities measured at 1 bar in different directions. According to the measurements, they reported the shale elastic symmetry as hexagonal (or transversely isotropic) with the symmetry axis normal to the bedding plane. The components of the stiffness tensor (in Voigt notation) found by Jones and Wang (1981) are $C_{11} = 34.3$, $C_{33} = 22.7$, $C_{44} = 5.4$, $C_{66} = 10.6$, and $C_{13} = 10.7$ (in GPa). The grain density is 2.59 g/cm³, and the bulk density measured in saturation conditions equals 2.42 g/cm³. The grain density has been measured with the air pycnometer on a sample heated to 80°C , thereby removing physically bound water and remaining chemically bound water in the lattice of the clay minerals. These two measurements of density provided the shale porosity of 11%.

Sayers (2005) considered the shale as a polycrystal consisting of anisotropic water-clay composites preferentially oriented in space. The stiffness tensor of the water-clay composite was inverted using the Voigt and Reuss averages from the distribution function (DF) of the clay platelets' orientation derived by Hornby et al. (1994) from a digitized SEM image of the Kimmeridge shale. It was impossible to derive the distribution function for the Greenhorn shale from the photos given by Jones and Wang because of their low resolution.

The elastic constants found by Sayers (2005) for the water-clay composite, which is a mixture of four different clays, are $C_{11} = 40.0$, $C_{33} = 16.8$, $C_{44} = 2.7$, $C_{13} = 9.0$, and $C_{66} = 13.1$ (in GPa). Unfortunately, Sayers (2005) did not mention how the silt minerals (quartz, feldspar, and pyrite) and porosity had been extracted from the shale; therefore, it is unclear if they were taken into account or were "left" in the water-clay composite.

In this paper, we derive the stiffness tensor of the water-clay mixture composite from the elasticity constants of the same sample of Greenhorn shale (from 5000-ft-depth) using the generalized singular approximation (GSA) method of effective media theory (Shermeger, 1977; Bayuk and Chesnokov, 1998). This method makes it possible to calculate the effective elastic properties depending on the rock's microstructure. The procedure includes several steps, and at each step the respective stiffness tensor is found with the help of a nonlinear optimization with bounds imposed on the sought-for parameters (the direct search complex algorithm included in the Microsoft Compaq Fortran Library, Version 6.6).

We use the Greenhorn shale sample for our modeling for the following reasons. Our inversion method requires information about all five independent constants of the shale's stiffness tensor (or about

velocities needed to derive the constants). In addition, the porosity and mineral composition (in volume or weight percent) of the shale should be known. Many authors reported measurements on shales; however, the data given are insufficient for the inversion. Kaarsberg (1959) perform an extensive study of the elastic waves in shales. He investigates the effect of the mineral composition, particle orientation, and interparticle adhesion on the relationship between P-wave velocity and density. He reports both compressional and shear wave velocities for angles of 0°, 45°, and 90° in the normal-to-bedding plane, which are sufficient to derive the shale stiffness tensor. However, neither porosity nor mineral composition was given (only minerals composing the shales were listed) in his work. Vernik and Nur (1992) and Wang et al. (2001) study many shales and presented the porosity and velocities measured at the three angles. Nonetheless, no information on the shale's mineral composition could be derived from these works.

METHOD

The method applied to find the stiffness tensor of the water-clay composite from the Greenhorn elasticity data, in some sense, can be considered as going in the “opposite direction” to the method used by Hornby et al. (1994) to theoretically calculate the effective stiffness tensor of the Greenhorn shale. Another major difference is that they used isotropic clay moduli for modeling, whereas our technique results in an anisotropic stiffness tensor of the water-clay composite.

The inversion of the tensor has been performed using the following steps (Figure 1). At the first step, we extract the silt minerals from the porous clay matrix (Figure 1a). This figure is taken from Hornby et al. (1994). Then, at the second step, we remove porosity from the clay matrix (Figure 1b). As a result, we have a polycrystal with preferentially oriented particles of water-clay composite (Figure 1c). At the third step, we follow Hornby et al. (1994) and apply the distribution function of clay platelets' orientation for the Kimmeridge shale to invert the stiffness tensor of the water-clay composite consisting of the four clay types (Figure 1d).

Methods of the effective medium theory

The methods of effective media theory (EMT) allow one to determine the physical properties (elastic, thermal, and electrical) of heterogeneous media at a given scale from the properties of components at a smaller scale. The medium at the smaller scale level should be statistically homogeneous. The greater scale should be large enough to calculate stable statistical characteristics of the properties from their distribution at the smaller scale.

As related to elasticity, the methods are applicable in the case when the wavelength is much greater than the inclusion sizes. At the scale of rock samples, this theory makes it possible to obtain the properties of samples from the properties of mineral grains and materials filling pores and cracks (so-called inclusions). In general, these methods are able to take into account the shape and orientation of inclusions (Eshelby, 1957; Hashin and Shtrikman, 1963; Budiansky, 1965; Willis, 1977; Shermegor, 1977; Nishizawa, 1982). Some methods even make it possible to take into account the spatial distribution of inclusions (Castaneda and Willis, 1995; Chesnokov et al., 1995).

In the EMT, the macroscopic properties of a heterogeneous medium are described by the effective stiffness tensor $\mathbf{C}^*$ that relates, via the Hook law, the strain ($\boldsymbol{\epsilon}$) and stress ($\boldsymbol{\sigma}$) fields averaged over the

representative volume (large enough compared to the heterogeneity size but small compared to the wavelength):

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{C}^* \langle \boldsymbol{\epsilon} \rangle. \quad (1)$$

In formula 1, the brackets $\langle \rangle$ mean averaging over the representative volume:

$$\langle \boldsymbol{\sigma} \rangle \equiv \frac{1}{V} \int_V \boldsymbol{\sigma}(\mathbf{r}) d\mathbf{r}, \quad \text{and} \quad \langle \boldsymbol{\epsilon} \rangle \equiv \frac{1}{V} \int_V \boldsymbol{\epsilon}(\mathbf{r}) d\mathbf{r}. \quad (2)$$

The quantities $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are the functions of point $\mathbf{r}$ within the representative volume V , but $\langle \boldsymbol{\sigma} \rangle$, $\langle \boldsymbol{\epsilon} \rangle$, and $\mathbf{C}^*$ are the constant tensors.

This problem of determination of effective properties is the so-called many-body problem (in terms of interactions of different portions of the medium). This problem can be solved, in the general case, only approximately. Different methods of EMT commonly produce different results for the same heterogeneous medium. In the derivation of all EMT methods, the principal goal is to find a linear relation between the local and average strain (or stress) field, i.e.,

$$\boldsymbol{\epsilon} = \mathbf{Q} \langle \boldsymbol{\epsilon} \rangle. \quad (3)$$

Once the tensor $\mathbf{Q}$ is found, the solution to the effective stiffness tensor is obtained as follows. Multiplying the left- and right-hand sides by the stiffness tensor $\mathbf{C}$ (which also depends on the point within the representative volume), we have

$$\boldsymbol{\sigma} = \mathbf{C} \boldsymbol{\epsilon} = \mathbf{C} \mathbf{Q} \langle \boldsymbol{\epsilon} \rangle. \quad (4)$$

Then, averaging over the representative volume, gives us

$$\langle \boldsymbol{\sigma} \rangle = \langle \mathbf{C} \mathbf{Q} \rangle \langle \boldsymbol{\epsilon} \rangle, \quad (5)$$

and according to definition 1, we obtain

$$\mathbf{C}^* = \langle \mathbf{C} \mathbf{Q} \rangle. \quad (6)$$

Irrespective of the simplicity of relation 6, the problem of determination of the tensor $\mathbf{Q}$ is very complicated. In general, the tensor

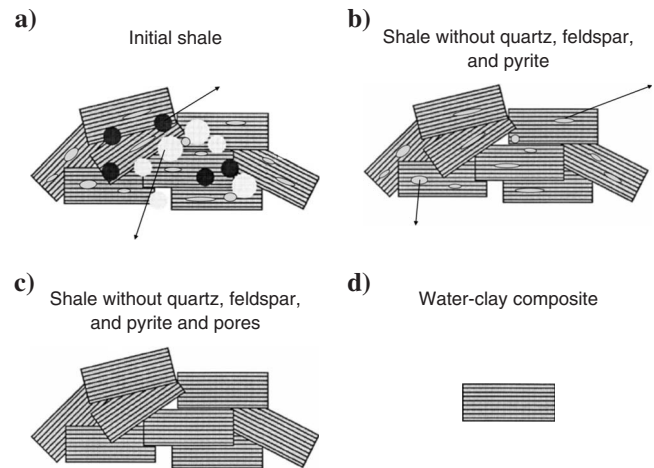


Figure 1. (a) Extraction of silt minerals from shale. The figure (without cracks) is taken from Hornby et al. (1994). (b) Extraction of pores from porous clay matrix; (c) water-clay polycrystal; (d) water-clay composite. Black and white spheres are silt particles, and gray ellipsoids are pores and cracks.

$\mathbf{Q}$ is not a constant tensor but an integral operator. However, various assumptions and simplifications make it possible to obtain a relation for $\mathbf{Q}$ in the form of a constant tensor.

The derivation of the relation between the local and average strain fields in the GSA method is based on a comparison of the strain fields in the heterogeneous body and in a homogeneous body with known properties (so-called comparison body), arising under the action of the same boundary conditions. The solution is found with the help of the Green function method and is based on decomposition of the Green function into the singular and regular terms. A detailed derivation of the formula of the GSA method is given in the work (Bayuk and Chesnokov, 1998) following the original derivation of Shermergor (1977). In this paper, we present another derivation of the GSA method formulas based on the well-known Eshelby solution (1957) for strain in an inclusion embedded into a matrix, arising under the action of an external field. The resulting relation between the local and average strain fields is found in the form (see Appendix A)

$$\boldsymbol{\epsilon}(\mathbf{r}) = [\mathbf{I} - \mathbf{g}\mathbf{C}'(\mathbf{r})]^{-1} \langle [\mathbf{I} - \mathbf{g}\mathbf{C}'(\mathbf{r})]^{-1} \rangle \langle \boldsymbol{\epsilon}(\mathbf{r}) \rangle, \quad (7)$$

where $\mathbf{I}$ is the fourth-rank unit tensor with the components

$$I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (8)$$

and δ_{ij} are the components of the Kronecker tensor. The tensor $\mathbf{C}(\mathbf{r}) \equiv \mathbf{C}(\mathbf{r}) - \mathbf{C}^c$ is the fluctuation of the stiffness tensor. The tensor $\mathbf{g}$ in equation 7 is independent of the position within the representative volume and is controlled by the properties of the comparison body and the inclusion shape. Tensor $\mathbf{g}$ has the form shown in Appendix A. Note that Willis (1977) obtained the relation between local and average strain fields similar to 7 using another approach for the derivation.

According to relations 3 and 7 connecting the local and average strain fields, we have

$$\mathbf{Q} = [\mathbf{I} - \mathbf{g}\mathbf{C}'(\mathbf{r})]^{-1} \langle [\mathbf{I} - \mathbf{g}\mathbf{C}'(\mathbf{r})]^{-1} \rangle^{-1}, \quad (9)$$

and from equation 6 for the effective stiffness tensor, we obtain

$$\mathbf{C}^* = \langle \mathbf{C}(\mathbf{r}) [\mathbf{I} - \mathbf{g}\mathbf{C}'(\mathbf{r})]^{-1} \rangle \langle [\mathbf{I} - \mathbf{g}\mathbf{C}'(\mathbf{r})]^{-1} \rangle^{-1}. \quad (10)$$

For statistically homogeneous media, volume averaging can be replaced by the statistical averaging. In this case, relation 10 for the effective stiffness tensor can be written in the form

$$\begin{aligned} \mathbf{C}^* = & \left\{ \sum_i v_i \mathbf{C}_i \int P_i(\chi_i; \theta, \varphi, \psi) \right. \\ & \times [\mathbf{I} - \mathbf{g}_i(\mathbf{C}_i - \mathbf{C}^c)]^{-1} \sin \theta d\chi_i d\theta d\varphi d\psi \left. \right\} \\ & \times \left\{ \sum_i v_i \int P_i(\chi_i; \theta, \varphi, \psi) \right. \\ & \times [\mathbf{I} + \mathbf{g}_i(\mathbf{C}_i - \mathbf{C}^c)]^{-1} \sin \theta d\chi_i d\theta d\varphi d\psi \left. \right\}^{-1} \quad (11) \end{aligned}$$

Here, v_i and $\mathbf{C}_i$ are, respectively, the volume concentration and stiffness tensor of the i th component.

In this modeling, we assume that inclusions have the shape of ellipsoids of revolution and, therefore, can be characterized by the as-

pect ratio χ . The aspect ratio is the ratio of the inclusion semiaxis normal to the symmetry plane to the semi-axis in the symmetry plane. The function P is the function of distribution of the inclusions' volume over their shape and orientations; θ, φ, ψ are the Eulerian angles describing the inclusion orientation in space.

Thus, the GSA method allows one to calculate the effective stiffness tensor depending on the volume concentration of inclusions (mineral grains, pores, and cracks), their shape, and orientation in space. The rock's microstructure can be also taken into account as shown below.

Choice of the comparison body

In the Eshelby-based derivation presented in Appendix A, the matrix plays the role of the comparison body. This choice of comparison body corresponds to the media of "matrix-inclusions" type when isolated inclusions are embedded in a matrix. If the matrix happens to be more compliant, we obtain the upper Hashin-Shtrikman bound; if the matrix is the stiffest phase, we have the lower Hashin-Shtrikman bound (Hashin and Shtrikman, 1963; Willis, 1977; Castaneda and Willis, 1995). All intermediate structures commonly met in reality are within these bounds. Considering a two-phase medium, namely, a porous-cracked medium, we use the following formula for the comparison body, it being a linear combination of matrix (m) and fluid (fl) properties:

$$\mathbf{C}^c = (1 - f)\mathbf{C}^m + f\mathbf{C}^n. \quad (12)$$

If fluid inclusions are isolated, the choice $f = 0$ in formula 12 gives the upper Hashin-Shtrikman bound. The other limiting choice, $f = 1$, produces the lower Hashin-Shtrikman bound corresponding to the case when fluid forms a single-connected domain and mineral grains are isolated. Choosing this comparison body in the Eshelby-based derivation, we place our inclusion in a medium with the properties defined by formula 12. Note that a similar principle was used by Hornby et al. (1994) for derivation of the self-consistent method formulas for porous-crack medium in which both fluid and solid phases are connected. They replaced the host matrix by a medium with the effective properties, i.e., $\mathbf{C}^c = \mathbf{C}^*$. However, this choice provides no possibility to take into account the degree of fluid connectivity. Note that the choice $\mathbf{C}^c = \mathbf{C}^*$ gives the formulas of the classical self-consistent method (Willis, 1977) commonly applied for calculating the effective properties of polycrystals.

The factor f is an empirical parameter reflecting a degree of crack connectivity. Commonly, this factor is found from the inverse problem solution. The factor f can be considered as a measure of pore/crack connection via fractures whose sizes are small compared to pores and cracks that contribute to porosity. The volume of these fractures in rock is assumed to be negligibly small. In what follows, we call this parameter friability. A similar comparison body was used by Xu and White (1996) for the Willis' formulas. Note that in the derivations of Shermergor (1977) and Willis (1977), no constraint is imposed on the choice of comparison body, which gives us a possibility to choose any comparison body for the effective property calculations.

We choose the GSA method for the inverse problem solution because of the fact that, among many theoretical methods, this method allowed us to obtain the closest fit of experimental and theoretical velocities for media with known pore/crack geometry (Bayuk and Chesnokov, 1998).

Choice of the distribution function over shape of inclusions

We take the Beta-distribution as the distribution function describing the distribution of the inclusions' volume over their aspect ratio. The Beta-distribution has the form

$$P(x) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1} \quad (\alpha > 0, \beta > 0), \quad (13)$$

and its shape is very flexible depending on its parameters. The function can have maxima in the domain of both very thin and very long fractures, and at some parameters it resembles the lognormal distribution observed in the experimental study of pore/crack shape in sedimentary rocks (Brodov et al., 1991). If $\alpha = \beta = 1$, the Beta-distribution transforms into the uniform distribution.

Step 1. Extraction of silt minerals from porous clay matrix

At this step, we apply formula 11 for the effective stiffness tensor of the previous section assuming that the shale is the medium of matrix-inclusions type. The matrix of the medium is porous clay, and the inclusions are silt minerals — quartz, feldspar, and pyrite. For feldspar, we assume albite. We assume that the silt minerals are represented by small isometric pieces of polycrystals having isotropic moduli. The latter are calculated from the stiffness tensors of respective minerals given by Ahrens (1995) with the help of the self-consistent method of EMT. The resulting elastic wave velocities and density for the polycrystals are $V_p = 6.01$ km/s, $V_s = 4.06$ km/s, and density = 2.65 g/cm³ for quartz; $V_p = 6.01$ km/s, $V_s = 3.29$ km/s, and density = 2.62 g/cm³ for albite; $V_p = 7.86$ km/s, $V_s = 5.0$ km/s, and density = 4.92 g/cm³ for pyrite.

To find the stiffness tensor of the porous clay matrix, we use the nonlinear optimization with bounds imposed on the unknown parameters (the direct search complex algorithm included in the Microsoft Compaq Fortran library). The functional to be minimized has the form

$$\Psi(C_{11}^m, C_{13}^m, C_{33}^m, C_{44}^m, C_{66}^m) = \sum_{ij} \left[\frac{C_{ij}^e - C_{ij}^t(C_{11}^m, C_{13}^m, C_{33}^m, C_{44}^m, C_{66}^m)}{C_{ij}^e} \right]^2 \quad (14)$$

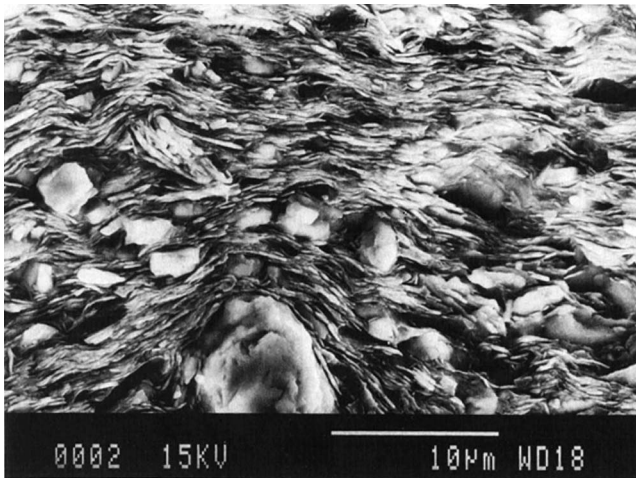


Figure 2. Scanning electron microphotograph of the Kimmeridge shale (taken from the work of Hornby et al. [1994]). The nearly spherical particles are silt, and thin particles are clay.

with the five unknown elastic constants C_{11}^m , C_{13}^m , C_{33}^m , C_{44}^m , and C_{66}^m of clay matrix with pores. The letters e and t mean, respectively, the elasticity constants obtained from experiment and calculated by formula 11. The pairs of indices ij correspond to the indices of five independent C_{ij} found from the experiment of Jones and Wang (1981). As many inverse problems in geophysics are not unique, physically plausible bounds imposed on the parameters allow one to obtain solution in a reliable domain. Thus, we assume that the elasticity constants of nonporous clay matrix are less than experimental values and positive. The parameters of the Beta-distribution function are selected to be positive, and the friability is supposed to vary within its specified limits — from 0 to 1.

The resulting constants of porous clay matrix are $C_{11} = 10.0$, $C_{33} = 6.0$, $C_{44} = 0.6$, $C_{66} = 2.3$, and $C_{13} = 4.3$ (in GPa).

Step 2. Extraction of pores from clay matrix

At this step, we again apply the EMT-based nonlinear optimization methods with bounds imposed on the sought-for parameters. The functional to be minimized in this case has the form similar to form 14 with C_{ij}^m characterizing elasticity of the nonporous clay matrix. For experimental values of elasticity constants, we take the constants found at the previous step (for the porous clay matrix). When solving the inverse problem, we apply different versions of the GSA method — the self-consistent method ($C^e = C^*$), the upper Hashin-Shtrikman bound ($C^e = C^m$), and the GSA method with $C^e = (1-f)C^m + fC^*$. The pore/crack shape is assumed to be specified by a single aspect ratio or by a distribution function of pore/crack volumes over their aspect ratio. The pore/crack orientation is assumed to be in accordance with the clay platelets' orientation found by Hornby et al. (1994) from the SEM image analysis of the Kimmeridge shale photo (Figure 2). The orientation of clay platelets in space computed from a digitized SEM image is presented in Figure 3. The distribution function has a shift around 6° from zero. We approximate this experimental histogram by the Gaussian distribution with the mean and standard deviation equal to 6° and 20° , respectively.

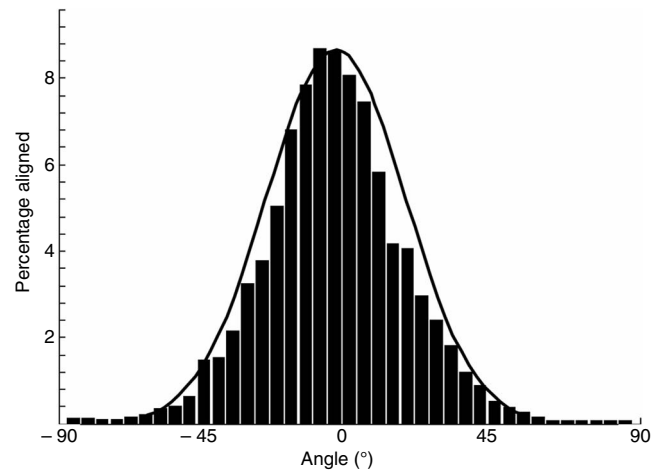


Figure 3. Approximation of experimental DF over clay platelets' orientation by the Gaussian DF (black curve) with zero mean and sigma equal to 20° . The experimental DF is obtained in the work of Hornby et al. (1994) from the SEM image of the Kimmeridge shale.

When modeling with a single aspect ratio, its value is assumed to be known and to be varying from 1/20 to 1/50. In this case, the friability is also fixed. When modeling with DF, the parameters of the Beta-function and friability are found from the optimization procedure. In this case, the minimized functional has the form

$$\Psi(C_{11}^m, C_{13}^m, C_{33}^m, C_{44}^m, C_{66}^m, f, \alpha, \beta) = \sum_{ij} \left[\frac{C_{ij}^e - C_{ij}^t(C_{11}^m, C_{13}^m, C_{33}^m, C_{44}^m, C_{66}^m, f, \alpha, \beta)}{C_{ij}^e} \right]^2 \quad (15)$$

in which the number of parameters to be determined is greater than the number of experimental values. This fact enhances nonuniqueness of the inverse problem solution. However, the bounds imposed on the sought-for parameters significantly restrict the domain of possible solutions.

Table 1. Elastic properties of nonporous clay matrix obtained with different versions of the GSA method.

Self-consistent method								
Aspect ratio of removed cracks	C_{11} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)	ϵ	γ	δ
1/20	11.4	5.1	7.4	1.4	2.7	0.27	0.46	0.07
1/30	11.3	5.1	7.4	2.0	2.6	0.26	0.15	0.27
1/50	11.3	5.2	7.4	4.4	2.6	0.26	-0.20	1.87
GSA, friability = 0 (upper Hashin-Shtrikman bound)								
Aspect ratio of removed cracks	C_{11} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)	ϵ	γ	δ
1/10	11.3	5.1	7.4	1.0	2.7	0.26	0.85	-0.04
1/20	11.3	5.1	7.5	1.3	2.6	0.25	0.5	0.03
1/30	11.2	5.2	7.5	1.8	2.6	0.25	0.22	0.19
1/50	11.2	5.2	7.6	2.9	2.6	0.24	-0.05	0.61
GSA, friability = 0.7								
Aspect ratio of removed cracks	C_{11} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)	ϵ	γ	δ
1/10	12.2	4.9	7.3	1.3	3.1	0.34	0.69	0.03
1/20	12.0	5.0	7.3	2.2	3.0	0.32	0.18	0.35
GSA, friability = 0.8								
Aspect ratio of removed cracks	C_{11} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)	ϵ	γ	δ
1/10	12.8	4.8	7.3	1.5	3.3	0.38	0.6	0.07
1/20	12.5	4.9	7.3	3.0	3.2	0.36	0.03	0.70

Table 1 presents the elasticity constants and the Thomsen parameters of the nonporous clay matrix inverted with the help of different GSA method versions. As seen, the most variable parameter is C_{44} . Other elasticity constants are rather stable with respect to both the aspect ratio chosen and the GSA method version used. As seen, the aspect ratio 1/50 provides unrealistic values of C_{44} and C_{66} with C_{44} greater than C_{66} , which results in negative γ . Note that the GSA method with fixed aspect ratio and friability gives no possibility to obtain solutions for an aspect ratio smaller than 1/20 with acceptable accuracy for the Greenhorn shale. When solving the inverse problem, we assume that the solution is acceptable if the difference between experimental and theoretical values of velocities does not exceed 0.5% (minimal experimental error in the Jones and Wang measurements). This means that the crack aspect ratio 1/50 is too low for the Greenhorn shale.

Table 2 presents two different solutions found for the case when the DF parameters and friability are found by minimizing functional 15. The two solutions for matrix C_{ij} differ insignificantly. An increase in friability increases the mineral matrix properties, since the greater the friability, the lower is the resulting elasticity moduli of porous/cracked rock. This means that in order to obtain the resulting stiffness tensor of porous/cracked shale for higher friability, the mineral matrix should be stiffer.

Figure 4 demonstrates the inverted distribution functions for pore/crack shape. The maxima of aspect ratio values are observed around 0.1. This rather large aspect ratio allows one to assume that the pores are generally concentrated in the vicinity of silt particles. This is in line with the SEM image of the Kimmeridge shale shown in Figure 2. We can consider the pores as grain-related pores.

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Step 3. Determination of elasticity constants of water-clay composite

At the final step, we assume that the nonporous clay matrix is a polycrystal containing clay platelets (with bound water) preferentially oriented in space. Hereinafter, we call the clay platelets with bound water the “water-clay” composite. The orientation of platelets is specified by the distribution function shown in Figure 3, obtained in the work of Hornby et al. (1994) for the Kimmeridge shale. In this case, the self-consistent method of EMT is applicable. The effective stiffness tensor of such a polycrystal is calculated by formula 11 in which we set $\mathbf{C}^e = \mathbf{C}^*$, $\nu = 1$ and $\chi = 1$.

The elasticity constants are found by minimizing functional 14 with experimental values of C_{ij} that are the elasticity constants of a nonporous clay matrix found at the previous step for the first solution of the inverse problem shown in Table 2 (friability = 0.78).

The inverted elasticity constants of the water-clay composite are $C_{11} = 24.6$, $C_{33} = 7.9$, $C_{44} = 0.5$, $C_{66} = 5.4$, and $C_{13} = 1.5$ (in GPa). Note that the elastic constants found for the second solution shown in Table 2 are very similar. The den-

sity of the composite found from the Greenhorn density and its mineral composition is 1.75 g/cm³. This value seems to be rather low. The reason of such a low value is that pyrite density is rather high, approximately 5.0 g/cm³, and pyrite occupies 9% of the shale volume.

We tried to analyze the reason for this low value of density. The grain density measured with an air pycnometer can be underestimated (K. Katahara, personal communication, 2006). Vernik and Liu (1997) use another value of density for the shale matrix, which averages 2.73 g/cm³. This value of grain density, gives porosity of 17% instead of 11% obtained with the grain density equal to 2.59 g/cm³ (the latter value is measured with the air pycnometer). We recalculate the elasticity moduli assuming that porosity is 17% and repeating all steps described above for the corrected porosity. The resulting moduli of the anisotropic water-clay composite are $C_{11} = 23.2$, $C_{33} = 8.5$, $C_{44} = 0.9$, $C_{66} = 5.6$, and $C_{13} = 3.1$ (in GPa); and density is 2.15 g/cm³. The distribution function of water-saturated voids removed at Step 2 is similar to that shown in Figure 3.

According to the results of Vernik (1994), at least 2% of kerogen is present in shales. There is no indication of the kerogen content for the Greenhorn shale, and this shale cannot be considered as kerogen-rich. Therefore, we take 2% of kerogen as a maximum value. Then, we solve the inverse problem on kerogen extraction from the clay moduli obtained at the last step found with the corrected porosity. The minimized functional has the form

$$\Psi(C_{11}^{cl}, C_{13}^{cl}, C_{33}^{cl}, C_{44}^{cl}, C_{66}^{cl}) = \sum_{ij} \left[\frac{C_{ij}^e - C_{ij}^t(C_{11}^{cl}, C_{13}^{cl}, C_{33}^{cl}, C_{44}^{cl}, C_{66}^{cl})}{C_{ij}^e} \right]^2, \quad (16)$$

where C_{ij}^{cl} are the components of the water-clay composite after kerogen extraction. When calculating the theoretical values of elasticity moduli, the matrix playing the role of the comparison body is assumed to be the kerogen material because kerogen surrounds the clay particles (Vernik, 1994). The elastic moduli of kerogen are taken as follows: V_p and V_s are 2.8 and 1.6 km/s, respectively, and density is 1.25 g/cm³ (Vernik and Liu, 1997). The minimization of functional 16 produces the following moduli of the anisotropic water-clay composite: $C_{11} = 23.7$, $C_{33} = 8.5$, $C_{44} = 0.8$, $C_{66} = 5.7$, and $C_{13} = 3.1$ (in GPa); and density equals 2.17 g/cm³.

DISCUSSION

Table 3 summarizes results of our inversion obtained at each step when assuming 17% porosity. The Thomsen parameters and bulk and shear moduli calculated with the self-consistent method for isotropic polycrystals are shown as well. For comparison, all these parameters are given for clay monocrystals of illite, kaolinite, and chlorite given by Alexandrov and Alexandrov and Ryzhova (1961). As seen, the presence of bound water increases the S-wave velocity anisotropy compared to the values observed for monocrystals because of lowered values of C_{44} in the water-clay composite.

To compare our results with the results of other authors who obtained the isotropic clay moduli, we calculate the elastic wave velocities of an isotropic polycrystal formed by randomly oriented particles of water-clay composite. The elasticity moduli of such a polycrystal are found by the formulas of the self-consistent method. The respective velocities of the isotropic water-clay composite are $V_p = 2.33$ km/s and $V_s = 1.13$ km/s with $V_p/V_s = 2.06$. Note that the VRH average produces very close velocities: 2.39 km/s and

1.14 km/s. Because a 2% kerogen content is only our assumption, we also calculate the velocities for shale without kerogen, i.e., for properties found before the kerogen extraction. The velocities for shale without kerogen are $V_p = 2.33$ km/s and $V_s = 1.16$ km/s, and $V_p/V_s = 2.00$. Thus, the 2% of kerogen added changed only the shear wave, decreasing it by 3%.

Table 4 lists the elastic wave velocities, moduli of elasticity, density, and V_p/V_s ratio for the water-clay composite under study and clays whose properties were found by different authors. The water-clay composite has elastic properties close to those of smectite found by Vanorio et al. (2003): $V_p = 2.3$ km/s, $V_s = 1.3$ km/s, and $V_p/V_s = 1.77$. Because of smaller shear wave velocity, the V_p/V_s ratio for the water-clay composite is greater, attaining 2.06. This is close to the V_p/V_s values reported by Castagna et al. (1985), Tosaya (1982), and Han et al. (1986). The velocities in clay containing equal amounts of illite and smectite should be greater than the velocities in pure smectite because illite absorbs less water. However, Vanorio et al. (2003) measured the velocities only in one direction of a cold-pressed sample — parallel to bedding. No measurements in the other directions were performed, but because of the anisotropic shape of the clay platelets, the sample also could be anisotropic and exhibit greater velocities in the bedding plane compared to the velocities calculated for an isotropic aggregate. Moreover, the smectite velocities in this work were obtained by the extrapolation of experimental values to zero porosity. To do this, the authors used the fourth-power polynomial, which also can give increased values.

Note that the elastic constants of the water-clay composite are

Table 2. Friability and elasticity constants of nonporous clay matrix provided by inversion based on the GSA method. The pore/crack shape is described by the Beta-distribution function.

Friability	C_{11} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)	ϵ	γ	δ
0.78	12.8	4.8	7.4	1.3	3.3	0.38	0.77	0.0
0.85	13.6	4.7	7.4	1.4	3.7	0.42	0.82	0.01

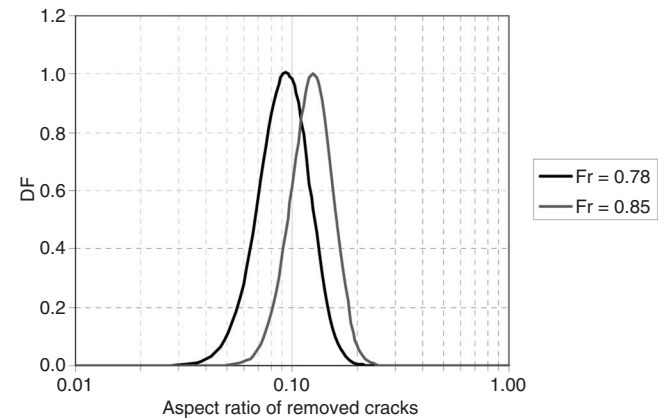


Figure 4. The functions describing distribution of pore/crack volume versus their aspect ratio in clay matrix at different friability values ($Fr = 0.78$ and $Fr = 0.85$).

Table 3. The elastic properties found at different steps of the inverse problem solution. Clay monocrystal properties are also given.

Step	C_{11} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{66} (GPa)	C_{13} (GPa)	K_{self} (GPa)	μ_{self} (GPa)	ϵ	γ	δ
Initial data (Jones and Wang, 1981)	34.3	22.7	5.4	10.6	10.7	17.4	7.7	0.33	0.48	-0.05
After removing silt minerals	10.0	6.0	0.6	2.3	4.3	5.7	1.3	0.33	1.42	-0.08
After extraction of pores from clay matrix (friability = 0.76)	14.4	8.5	1.8	3.8	5.3	7.7	2.6	0.35	0.56	0.05
Elasticity constants of water-clay composite before kerogen removal	23.2	8.5	0.9	5.6	3.1	7.8	2.9	0.86	2.61	-0.31
Elasticity constants of water-clay composite after kerogen removal	23.7	8.5	0.8	5.7	3.1	8.1	2.8	0.89	3.10	-0.34
Clay monocrystals										
Illite (Alexandrov and Ryzhova, 1961)	179.9	55.0	11.7	70.0	14.5	52.3	31.7	1.13	2.49	-0.25
Kaolinite (Alexandrov and Ryzhova, 1961)	171.5	52.6	14.8	66.3	27.1	55.5	31.8	1.13	1.75	0.08
Chlorite (Alexandrov and Ryzhova, 1961)	181.8	106.8	11.4	62.5	20.3	54.3	30.2	0.35	2.24	-0.40

Table 4. Isotropic elastic properties of clays.

Clay	K (GPa)	μ (GPa)	ρ (g/cm ³)	V_p (km/s)	V_s (km/s)	V_p/V_s	Method used	Reference
Illite	52.3	31.7	2.79	5.82	3.37	1.73	VRH averaging	Katahara, 1996
Chlorite	54.3	30.2	2.69	5.93	3.35	1.77	-----"	-----"
Kaolinite	55.5	31.8	2.52	6.23	3.55	1.75	-----"	-----"
Motmorillonite-illite mixture				3.60	1.85	1.95	Extrapolation of empirical dependences to pure clay	Castagna et al., 1985
Mixed clays				3.40	1.60	2.13	-----"	Tosaya, 1982
Mixed clays	21.4	6.7	2.62	3.41	1.63	2.09	-----"	Han et al., 1986; Berge and Berryman, 1995
Illite				4.2	2.5	1.68	-----"	Eastwood and Castagna, 1986
Smectite	7.0	3.9	2.29	2.30	1.30	1.77	Measurements on cold-pressed sample	Vanorio et al., 2003
Kaolinite	12.0	6.0	2.59	2.78	1.52	1.83	Measurements on clay-water suspension, AFAM	Vanorio et al., 2003 Prasad et al., 2002
Illite	60.2	25.4	2.71	5.89	3.06	1.92	Inverted from clay-epoxy mixture properties	Wang et al., 2001
Smectite	9.3	6.9	2.40	2.78	1.70	1.63	-----"	Wang et al., 2001
Illite-smectite mixture (60/40)	37.0	18.2	2.55	4.90	2.67	1.84	-----"	Wang et al., 2001
Kaolinite	44.3	22.1	2.44	5.50	3.01	1.83	-----"	Wang et al., 2001
Kaolin (rock or mineral?)	1.4	1.4	1.58	1.44	0.93	1.55	Measurements on cubic sample	Woeber et al., 1963
Illite-smectite-kaolinite-chlorite mixture	8.1	2.8	2.17	2.33	1.13	2.06	Inversion from Jones and Wang data (1981) and calculations with the self-consistent method	This study
Illite-Smectite-Kaolinite-Chlorite mixture	16.0	6.4	2.17	3.36	1.76	1.91	Inversion from Jones and Wang data (1981) and calculations with the self-consistent method	Sayers, 2005

found for clay having the composition inherent in the Greenhorn shale. Illite and smectite occupy almost the same volume. The elasticity constants derived can be used for modeling of elastic anisotropy in shales composed mostly of smectite and illite and having comparable amounts of both. For other shales, having another clay composition, the elasticity constants of a water-clay composite can be different. Our approach can be used to determine the elasticity constants of a water-clay composite for various relative contents of clay minerals.

CONCLUSIONS

We have developed a technique allowing one to determine the stiffness tensor of in situ clay (water-clay composite) from the shale stiffness tensor, its mineral composition, and information on clay platelets orientation. The technique is the EMT-based step-by-step inversion of stiffness tensors of the following media: (1) shale without silt, (2) shale without silt and pores, (3) clay aggregate with different orientation of in situ clay particles (particles of water-clay composite), (4) and finally, water-clay composite.

This technique has been applied to find the components of the stiffness tensor of an in situ water-clay composite composed of almost equal amounts of illite and smectite (36% and 34%, respectively) and similar amounts of kaolinite and chlorite (17% and 13%, respectively). The parameters found are in correspondence with data on in situ clay elasticity presented by other authors for isotropic clay aggregates. The results are useful for theoretical modeling of elasticity of shales having similar clay composition.

The technique developed can be used to determine the stiffness tensor of in situ clay of any composition from shale for which the stiffness tensor, mineral composition, and orientation of clay platelets are known.

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APPENDIX A

DETERMINATION OF THE RELATION BETWEEN LOCAL AND AVERAGE STRAIN FIELDS IN A MEDIUM WITH ELLIPSOIDAL INCLUSIONS

Eshelby (1957) solve a problem on determination of the strain field in an individual ellipsoidal inclusion embedded in a homogeneous matrix with other elastic properties, which is caused by a field applied at infinity. The elastic properties of matrix and inclusion can be anisotropic. The inclusion shape is ellipsoidal. We briefly repeat here the steps of the Eshelby solution and find a relation between the local and averaged strain fields in the case when medium contains many ellipsoidal inclusions.

Step 1. At this step, we consider the matrix and inclusion free of action of any external forces. We remove the inclusion from the matrix and replace it by an inclusion of the same shape but having the properties of matrix. Then, deform the inclusion such that the strain

in the inclusion is ϵ^T , but stress is zero (we imagine that this could be done).

Step 2. We apply the following forces on the inclusion surface:

$$-\sigma_{ij}^T n_j = -C_{ijkl}^M \epsilon_{kl}^T n_j, \quad (\text{A-1})$$

where C_{ijkl} are the components of the stiffness tensor of matrix, and n_j are the components of the normal to the inclusion surface. As a result, the inclusion restores its shape. Then, we embed the inclusion back into the matrix, at its previous place, and “glue” the material on the matrix-inclusion interface S . The resulting material is continuous, and each point is at the place where it was before the inclusion removal. After this step, the stress field in the matrix is zero, but in the inclusion, the stress field is $-\sigma^T$.

Step 3. We stop to apply the forces to the inclusion surface necessary for keeping its shape. This is the same as if we apply to its surface the compensating forces $+\sigma^T n_j$. These forces cause the strain ϵ^c both in the inclusion and in the matrix. The respective stress is $\sigma^c = C^M \epsilon^c$. After this step, the stress in the matrix and inclusion are, respectively, σ^c and $\sigma^c - \sigma^T$.

To calculate the stress $\epsilon_{ij}^c = (u_i^c + u_j^c)/2$, where $\mathbf{u}$ is the displacement, we apply the Green function. As a result we have

$$u_m(\mathbf{r}) = \int_V \mathbf{G}_{im}(\mathbf{r} - \mathbf{r}_1) f_i(\mathbf{r}_1) d\mathbf{r}_1 + \int_S [u_i(\mathbf{r}_1) C_{ijkl} \mathbf{G}_{km,l} \times (\mathbf{r} - \mathbf{r}_1) + \mathbf{G}_{im}(\mathbf{r} - \mathbf{r}_1) \sigma_{ij}(\mathbf{r}_1)] dS_{1j}, \quad (\text{A-2})$$

where f_i are the components of the density of volume forces, and $\mathbf{G}$ is the Green function, which is a tensor. This is the common expression for a body of the volume V and surface S (Mura, 1991); $\mathbf{r}$ and $\mathbf{r}_1$ are the points in the volume V and on the surface S .

After this step, the volume forces are zero (we neglect the gravity). The conditions on the inclusion surface are $\sigma^T = \text{const}$, and the displacements on its surface are zero. This gives

$$u_i^c(\mathbf{r}) = \int_S \sigma_{ik}^T \mathbf{G}_{il}(\mathbf{r} - \mathbf{r}_1) dS_{1k} = - \sigma_{ik}^T \int_V \mathbf{G}_{il,k}(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1. \quad (\text{A-3})$$

Going from the displacement to the strain field, we can write

$$\begin{aligned} \epsilon_{mn}^c(\mathbf{r}) &= [u_{m,n}(\mathbf{r}) + u_{n,m}(\mathbf{r})]/2 \\ &= -C_{klij}^M \epsilon_{ij}^T \left[\int_V \mathbf{G}_{ml,kn}(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1 \right. \\ &\quad \left. + \mathbf{G}_{nl,km}(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1 \right] / 2. \end{aligned} \quad (\text{A-4})$$

Here we take into account that only the Green function depends on the coordinates.

Introducing the tensor (which is called the Eshelby tensor)

$$T_{mnij}(\mathbf{r}) = -C_{klij}^M \int_V \left[\frac{\mathbf{G}_{km,ln}(\mathbf{r} - \mathbf{r}_1) + \mathbf{G}_{kn,lm}(\mathbf{r} - \mathbf{r}_1)}{2} \right] d\mathbf{r}_1, \quad (\text{A-5})$$

we have

$$\epsilon^c = \mathbf{T} \epsilon^T. \quad (\text{A-6})$$

In relation A-5, comma means that the derivatives are taken with respect to coordinates following the comma. Thus, the first term in the right-hand side of relation A-5 contains the second derivatives of the Green function with respect to l and n , and the second term contains the derivatives with respect to l and m . Integration in formula A-5 is performed over the inclusion volume. We introduce the notation

$$a_{iklm}(\mathbf{r}) \equiv \int_V \mathbf{G}_{ik,lm}(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1 \text{ and} \\ g_{kmln}(\mathbf{r}) \equiv \frac{(a_{kmln} + a_{knlm})}{2}. \quad (\text{A-7})$$

Then, the Eshelby tensor can be written in the form

$$T_{imjn}(\mathbf{r}) = -C_{klij}^M g_{kmln}(\mathbf{r}). \quad (\text{A-8})$$

It was shown by Kinoshita and Mura (1971), Shermegor (1977), and Mura (1991) that, for an ellipsoidal inclusion, the tensor $\mathbf{a}$ can be written in the form

$$a_{imjn} = -\frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} n_{mn} \Lambda_{ij}^{-1} d\Omega, \quad (\text{A-9})$$

where $\Lambda_{ij} \equiv C_{imjn}^M n_{mn}$, $n_{mn} \equiv n_m n_n$, $n_1 = \frac{\sin \theta \cos \varphi}{a_1}$, $n_2 = \frac{\sin \theta \sin \varphi}{a_2}$, $n_3 = \frac{\cos \theta}{a_3}$, and $d\Omega \equiv \sin \theta d\theta d\varphi$. Here, a_1 , a_2 , and a_3 are the semiaxes of ellipsoidal inclusion. As seen from formula A-9, in the case of ellipsoidal inclusion, the tensor $\mathbf{a}$ is constant, and the Eshelby tensor $\mathbf{T}$ is constant as well.

According to relations A-8 and A-9, the Eshelby tensor is controlled by the elastic properties of the host matrix and the shape of the inclusion.

Step 4. We apply a homogeneous external strain ϵ^A on the matrix-inclusion system. In this case, the strain on the inclusion's surface is $\epsilon^C + \epsilon^A$, and the strain within the inclusion is $\epsilon^C + \epsilon^A - \epsilon^T$. Note that ϵ^T is still arbitrary. We replace now the inclusion having the matrix properties by the initial inclusion with the properties $\mathbf{C}'$ such that the stress fields in the system matrix-inclusion will not change. In this case, the stress in the inclusion having the properties $\mathbf{C}'$ should obey the condition

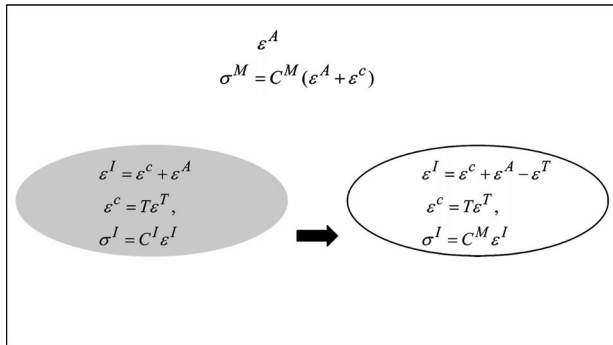


Figure A-1. The distribution of strain and stress fields in the matrix, original inclusion (light ellipsoid), and replacing inclusion (dark ellipsoid) at step 4 of the Eshelby-based solution. Black arrow indicates the replacement of inclusion having the matrix properties by the original inclusion. For notation see the text.

$$\sigma^I = \mathbf{C}' \epsilon^I = \mathbf{C}' (\epsilon^C + \epsilon^A) = \sigma^M = \mathbf{C}^M (\epsilon^C + \epsilon^A - \epsilon^T). \quad (\text{A-10})$$

The distribution of strain and stress fields in the matrix and in the inclusions and matrix at step 4 is shown in Figure A-1.

From equation A-10, the solution for ϵ^T is found in the form

$$\epsilon^T = -[(\mathbf{C}^M - \mathbf{C}')\mathbf{T} - \mathbf{C}^M]^{-1}(\mathbf{C}^M - \mathbf{C}')\epsilon^A. \quad (\text{A-11})$$

In derivation of formula A-11, relation A-6 between the strains ϵ^T and ϵ^C is used.

Substituting relation A-11 for the strain ϵ^T into formula A-6, we have

$$\begin{aligned} \epsilon^C &= \mathbf{T}[(\mathbf{C}^M - \mathbf{C}')\mathbf{T} - \mathbf{C}^M]^{-1}(\mathbf{C}' - \mathbf{C}^M)\epsilon^A \\ &= \mathbf{T}[(\mathbf{C}^M - \mathbf{C}')\mathbf{T} - \mathbf{C}^M \mathbf{T}^{-1} \mathbf{T}]^{-1}(\mathbf{C}' - \mathbf{C}^M)\epsilon^A \\ &= [(\mathbf{C}^M - \mathbf{C}') - \mathbf{C}^M \mathbf{T}^{-1}]^{-1}(\mathbf{C}' - \mathbf{C}^M)\epsilon^A. \end{aligned} \quad (\text{A-12})$$

Using relation A-12, we obtain the following formula for the strain field in the inclusion with the properties $\mathbf{C}'$:

$$\epsilon^I = \epsilon^C + \epsilon^A = [\mathbf{I} - (\mathbf{C}' + \mathbf{C}^M \mathbf{T}^{-1})^{-1} \mathbf{C}']\epsilon^A, \quad (\text{A-13})$$

where $\mathbf{C} \equiv \mathbf{C}' - \mathbf{C}^M$.

Substituting equation A-8 for the Eshelby tensor into formula A-13, we obtain

$$\begin{aligned} \epsilon^I &= [\mathbf{I} - (\mathbf{C}' - \mathbf{g}^{-1})^{-1} \mathbf{C}']\epsilon^A \\ &= [(\mathbf{C}' - \mathbf{g}^{-1})^{-1}(\mathbf{C}' - \mathbf{g}^{-1}) - (\mathbf{C}' - \mathbf{g}^{-1})^{-1} \mathbf{C}']\epsilon^A \\ &= (\mathbf{C}' - \mathbf{g}^{-1})^{-1}(\mathbf{C}' - \mathbf{g}^{-1} - \mathbf{C}')\epsilon^A \\ &= (\mathbf{g}^{-1} - \mathbf{C}')^{-1} \mathbf{g}^{-1} \epsilon^A \\ &= (\mathbf{I} - \mathbf{g} \mathbf{C}')^{-1} \epsilon^A. \end{aligned} \quad (\text{A-14})$$

Equation A-14 relates the strain field in the inclusion and the applied strain ϵ^A . As seen, in the case of an ellipsoidal inclusion, the strain field is constant if the applied strain is constant as well.

We assume now that many inclusions are embedded in the matrix, and the resulting medium is statistically homogeneous. Using equation A-14 and supposing that a contribution of inclusion-inclusion interaction into the local strain field is small, we find the strain field averaged over all inclusions in the form

$$\langle \epsilon \rangle = \langle (\mathbf{I} - \mathbf{g} \mathbf{C}')^{-1} \rangle \epsilon^A, \quad (\text{A-15})$$

which gives

$$\epsilon^A = \langle (\mathbf{I} - \mathbf{g} \mathbf{C}')^{-1} \rangle^{-1} \langle \epsilon \rangle. \quad (\text{A-16})$$

Substituting relation A-16 into formula A-14 for ϵ^I , we obtain the relation between the strain in the inclusion and average strain in the form

$$\epsilon^I = (\mathbf{I} - \mathbf{g} \mathbf{C}')^{-1} \langle (\mathbf{I} - \mathbf{g} \mathbf{C}')^{-1} \rangle^{-1} \langle \epsilon \rangle \quad (\text{A-17})$$

or

$$\epsilon(\mathbf{r}) = [\mathbf{I} - \mathbf{g} \mathbf{C}'(\mathbf{r})]^{-1} \langle [\mathbf{I} - \mathbf{g} \mathbf{C}'(\mathbf{r})]^{-1} \rangle^{-1} \langle \epsilon \rangle, \quad (\text{A-18})$$

where $\mathbf{r}$ is assumed to be constant within the ellipsoidal inclusion.

Equation A-18 can be used for derivation of a formula to allow calculation of the effective stiffness tensor.

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