Computational study of the elastic behavior of the $2M_1$ muscovite-paragonite series

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ABSTRACT

Elastic properties are an important issue in explaining the behavior of seisms and to ascertain the mineralogical composition of the Earth’s shells through which seismic waves pass. Computational methods can yield an additional, detailed, free-of-heterogeneity model knowledge of the mineral series of interest. Therefore, a computational study on the influence of the interlayer cation in the muscovite-paragonite (Ms-Pg) series on the crystal cell, internal geometry, and the elastic properties was made to shed light on the mineralogical, geophysical, and geochemical properties of the series. These properties have been calculated by means of Density Functional Theory (SIESTA2.0.2 code). The crystal structure and internal geometry agreed with the range of experimental values in the literature. In general, elastic stiffness constants (EC) agreed with the known experimental values. ECs of different interlayer cation configurations for the middle concentration sample showed very similar values, except for $C_{33}$. The majority of ECs, with the exception of $C_{13}$ and $C_{66}$, decreased as a function of Na’ [$Na/(Na+K)$], many of which showed ideal crystalline solution behavior, and some showed mixing terms. The polycrystalline bulk modulus registered similar values for the end-members of the series and a minimum at Na’ = 0.5, although an estimate of the value at room temperature made the Pg stiffer than Ms; while the shear modulus showed a decreasing trend as a function of the Na’. Velocities of the sound waves lowered as a function of Na’. Local deformabilities were also studied, where the highest deformability was found for the interlayer space. The results are discussed in the framework of the mineralogical, geochemical, and geophysical knowledge of the series.

Keywords: Muscovite-paragonite series, crystal structure, local geometries, elastic-stiffness constants, bulk and shear moduli, local deformabilities, DFT calculations

INTRODUCTION

Velocities of earthquake-generated acoustic waves are determined by the elastic properties of the materials they pass through, and from these two parameters it is possible to account for the structure, compositions and dynamics of the Earth’s shells. Thus, although the elastic properties of minerals are key geophysical data, it is frequently difficult to measure the exact elastic-stiffness constants (ECs), especially in natural minerals where cation order/disorder, morphological, crystal-chemical, and crystal-physical heterogeneities exist (Mondol et al. 2008). However, computational methods can yield reliable crystal structures and ECs free of these natural heterogeneities (Karki et al. 2001; Stixrude 2002; Stixrude and Peacor 2002; Weirich 2004; Ortega-Castro et al. 2010; Militzer et al. 2011). This can help explain the crystal-chemical, crystal-physical, mineralogical, and petrological behavior of minerals and aid interpretations of the seismologic data.

Phyllosilicates, found in the Earth’s crust and even in the upper mantle, are also found in subduction slabs in a wide compositional range, depending on the pressure ($P$), temperature ($T$), and composition of the bulk rock. Micas are 2:1 phyllosilicates (21P) (Moore and Reynold 1989), and because of many different cation substitutions form a major group of minerals. Micas are also one of the sources of water in the deep subduction zones.

Because of their high-chemical stability, micas have major industrial applications and include properties of films measuring several micrometers. Elastic, tough, and thermally resistant, micas have high-dielectric strength, so that they are valuable in industries related to optics and electricity. Micas show a wide compositional formula, which allows the tuning of some of their properties depending on the composition.

Muscovite (Ms) $[KAl_2(Si_OH)_{6}(OH)_2]_0$ is a dioctahedral mica, one of the most common and abundant minerals in metamorphic rocks (metapelites, shales, micaschists, gneiss, metabasites, etc.) and considered a useful petrogenetic indicator (Comodi and Zanazzi 1997). Ms is an end-member of the Ms-paragonite solvus. Paragonite (Pg) is the ideal end-member of the series with Na’ instead of K’ as an interlayer cation. This series has substitutions on the octahedral (Oc or VI) sheet, particularly Ms, which can undergo the substitution of $\text{Fe}^{3+}$, $\text{Fe}^{2+}$, and $\text{Mg}^{2+}$, yielding celadonite and phengite series; in addition, different $\text{Al}^{3+}$ substitutions also take place on the tetrahedral (T or IV) sheet. Phengitic Ms are stable at very high pressures in mature subduction zones, and they may be an important factor...