American Mineralogist, Volume 99, pages 1360–1368, 2014

First-principles elasticity of monocarboaluminate hydrates

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Abstract

The elasticity of monocarboaluminate hydrates, $3CaO \cdot Al_2O_3 \cdot CaCO_3 \cdot xH_2O$ (x = 11 or 8), has been investigated by first-principles calculations. Previous experimental study revealed that the fully hydrated monocarboaluminate (x = 11) exhibits exceptionally low compressibility compared to other reported calcium aluminate hydrates. This stiff hydration product can contribute to the strength of concrete made with Portland cements containing calcium carbonates. In this study, full elastic tensors and mechanical properties of the crystal structures with different water contents (x = 11 or 8) are computed by first-principles methods based on density functional theory. The results indicate that the compressibility of monocarboaluminate is highly dependent on the water content in the interlayer region. The structure also becomes more isotropic with the addition of water molecules in this region. Since the monocarboaluminate is a key hydration product of limestone added cement, elasticity of the crystal is important to understand its mechanical impact on concrete. Besides, it is put forth that this theoretical calculation will be useful in predicting the elastic properties of other complex cementitous materials and the influence of ion exchange on compressibility.

Keywords: Elasticity, ab initio calculations, crystal structure, monocarboaluminate