



Does the Al substitution in C–S–H(I) change its mechanical property?

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ABSTRACT

This study examines the influence of Al substitution for Si on the bulk modulus of calcium silicate hydrate I [C–S–H(I)], a structural analogue of C–S–H, by performing high-pressure synchrotron X-ray diffraction experiments in two C–S–H(I) samples: one a hydration product of alkali-activated slag and the other a synthetic C–S–H(I). The test result shows that not only the bulk modulus but also the incompressibility of the lattice parameters a , b , and c of two C–S–H(I) samples are very similar to each other, regardless of the Al substitution. This result may be due to the four-coordinated configuration of the substituted Al, which makes the dreierketten silicate chains maintain the same arrangement after the substitution.

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1. Introduction

There is a general agreement that the main reaction product of alkali-activated slag cement (AAS) is calcium silicate hydrate (C–S–H); however, it has a much lower Ca/Si ratio ($=0.8\sim1.5$) and is more crystalline than the C–S–H found in hydrated portland cement paste [1], consequently implying that the main reaction product of AAS is C–S–H(I) [2,3].

Besides its importance as a reaction product of AAS, C–S–H(I) has also gained significance in fundamental research because it has been viewed as an imperfect form of tobermorite in the C–S–H structural model [1]; that is, both C–S–H(I) and tobermorite resemble C–S–H with respect to their crystal structure [hereafter, we will call the chemically synthesized C–S–H(I) as SYN C–S–H(I) to distinguish the C–S–H(I) from AAS, which will hereafter be called AAS C–S–H(I)].

The major structural difference between SYN C–S–H(I) and AAS C–S–H(I) is the Al substitution for Si [frequently observed in AAS C–S–H(I)], which occurs predominantly at the bridging tetrahedral sites in dreierketten silicate chains in AAS (see Fig. 1), as confirmed by NMR studies [3–8].

The presence of other minor reaction products largely varies, depending on the sources of blast furnace slag and the types of alkali-activating solutions. Common minor reaction products include the hydrotalcite-like phase, the Fe-rich hydrogarnet phase, and the ettringite, $\text{Ca}(\text{OH})_2$, and AFm phases [3–5,9]. The hydrotalcite-like phase has been found to coexist intermixed with AAS C–S–H(I) and

has an approximate atomic ratio of Mg/Al = 2.1 [3], 2.55 [5], or 2.3 [10] although a theoretical atomic Mg/Al ratio of hydrotalcite [$\text{Mg}_6\text{Al}_2\text{CO}_3(\text{OH})_{16}\cdot 4\text{H}_2\text{O}$] is 3.0. Thus, some portion of Al found in AAS C–S–H(I) phase is consumed by the hydrotalcite-like phase and should be excluded in the calculation of Al/Si ratio in AAS C–S–H(I).

Earlier studies have reported atomic Al/Si ratios (or Al/Ca) in AAS C–S–H(I) as 0.11–0.34, which seems to be somewhat independent of hydration time [3,5,6,10–12]. The dreierketten silicate chains in C–S–H and C–S–H(I) resemble the long chains of tobermorite (see Fig. 1); however, the chains form fragments having 2, 5, 8, ..., $(3n-1)$ tetrahedra [1]. In real C–S–H, the dimers are the most predominant silicate chains [13], whereas in AAS C–S–H(I) and SYN C–S–H(I), pentamers are the most dominant chains [5,6,14]. When we assume that only pentameric silicate chains exist in AAS C–S–H(I) and Al substitution occurs dominantly at middle bridging tetrahedral sites, the value Al/Si = 0.11 in AAS C–S–H(I) indicates that approximately 50% of bridging tetrahedral sites are taken by tetrahedral Al atoms, and the Al/Si = 0.25 implies 100% of substitution of Al for bridging Si. Therefore, the Al/Si ratio = 0.11–0.34 indicates a high degree of Al substitution ratio in the AAS C–S–H(I) structure.

No study has investigated a possible change of the mechanical properties of C–S–H(I) attributed to the Al substitution although many papers discussed the Al substitution in AAS C–S–H(I) [3,5–7]. This study presents bulk modulus values of two different C–S–H(I) samples [i.e., SYN C–S–H(I) and AAS C–S–H(I)] using high-pressure synchrotron X-ray diffraction and discusses the effect of Al substitution on the bulk modulus of C–S–H(I). Note that AAS C–S–H(I) was a real hydration product and its hardened AAS paste showed a compressive strength of 49 MPa at 14 days of curing. Accordingly, the measured bulk modulus of AAS C–S–H(I) of the current study can

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