Polymorphs in Calcium Silicates Involved in Cement Chemistry

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The understanding of calcium silicates is crucial not only for minerals but for cement industry. On the one hand, calcium silicates show a number of polymorphs at certain compositions, such as tricalcium silicate and dicalcium silicate also known as alite and belite, respectively. These polymorphs have distinct physical and chemical properties related to the several structures as the temperature changes. Note that in industry the key polymorphs for both alite and belite are brought to work within the room temperature range by chemical doping, and their production is responsible of around 10% of anthropogenic CO_2 emission. On the other hand, these calcium silicates after hydration become inosilicates like tobermorite entering in the hydrated cement paste as the C-S-H gel which is the glue between cement grains. The tobermorite structure has calcium oxide layers ribbed with silicate chains, and several polymorphs are present according to the distance between these layers. For instance, tobermorite has three distinct structural varieties separated by 9, 11 and 14 Amstrongs.[1]

In this talk we consider firstly the stability of polymophs in dicalcium silicates using atomistic calculations. Furthermore in order to look at the transitions among the belite phases we describe the role of temperature looking at their phonon spectra and free energies [2]. In the second part, we focus on tobermorite because is the main compound obtained after the hydration of these calcium silicates. We investigate the role of having short silicate chains in the tobermorite phases, in agreement with the characterization s by nuclear magnetic resonance experiments [3]. Then we dope tobermorite with few percent of aluminum [4]. We recently found that aluminum has to replace silicon in the chains breaking Lowestein rules. This finding is relevant in order to understand why the transition between the tobermorite polymorphs doped with aluminum would happen to higher temperatures and pressures.

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