Poster

Structure relations of belite and alite polymorphs

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In the context, of the contribution of cement industry to the greenhouse effect there is an increased interest for using clinkers containing polymorphs of the main phases which are formed at lower temperatures, as this results in reduced gas emissions. Thus, any study that helps to explore the structure relations of the polymorphs present in the clinker is of interest for both scientific and practical point of view. O'Keefe & Hyde [1a,1b] use a description for non-molecular structures which is based on the arrangement of cations. This approach gives a simpler pattern for the arrangement of atoms in the structures and is an alternative to the usual description of polyhedra based on anions and introduced by Pauling [2]. Especially in the case of ternary oxides with two different metals the packing of cations resembles the packing of cations in their respective alloys. In a recent publication the structure-superstructure relations of Belite polymorphs have studied by our group [3] In the present work the structure relations of the polymorphs of alite (tricalcium silicate, Ca_3SiO_5) the major cement phase (>70% exists in the clinker), will be discussed. The complications related to the various ways of structure description for the seven polymorphs of Alite have been discussed in reference [4]. Our description uses the octahedra formed by Ca^{2+}, which were discussed for first time in [5], and following the ideas of O'Keefe & Hyde, gives a clearer picture for the structures of alite polymorphs and for their structure-relations as well. The common characteristic of all alite polymorphs is the fact that triplets of Ca^{2+} octahedra sharing faces exist in all of them and then neighbouring triplets by sharing corners the rhombohedral skeleton of their structures is formed. This description makes also clear the suggestion given in [6], that tricalcium silicate has to be considered as tricalcium oxy silicate. In the light of this findings the structures and properties relations of belite and alite phases will be discussed.

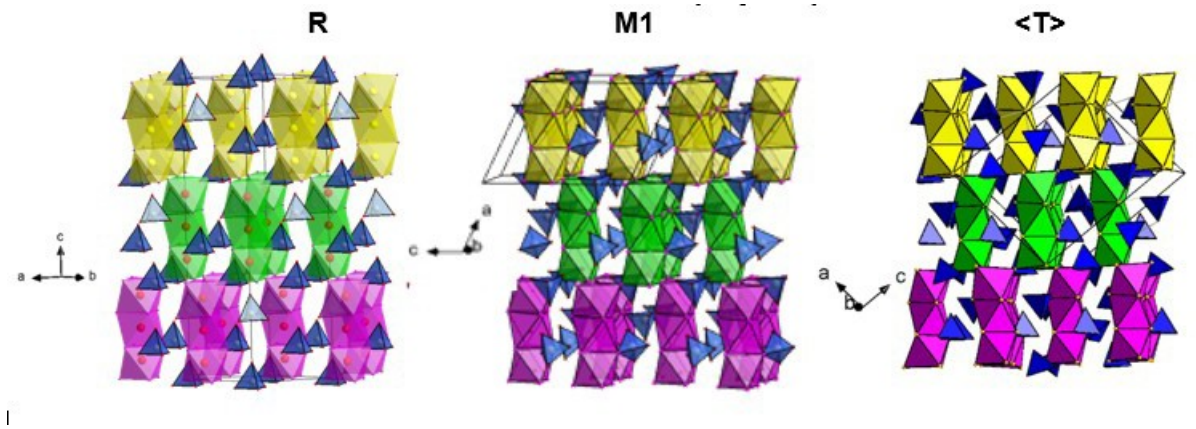

Figure 1. The rhombohedral skeleton of face sharing Ca^{2+} octahedra in Tricalcium Silicate polymorphs .

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[5] Dent Glasser, Acta Cryst., 1965, 18, 455-457

[6] Plank J., Cement and Concrete Research. 2020, 130, 105957.