Thermodynamic data of cement phases

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Enthalpy of formation and standard entropy data of some phases relevant in cement industry were acquired in this study.

Heat of dissolution data of calcium aluminate monocarbonate hydrate ($3CaO{\cdot}Al_2O_3{\cdot}CaCO_3{\cdot}10.7H_2O$), a typical hydration product of cement, briefly monocarbonate (MC) were obtained by acid solution calorimetry using an IMC 4400 isothermal microcalorimeter (Calorimetry Science Corporation) [1]. Low-temperature heat capacity data were recorded by relaxation calorimetry using a PPMS (Quantum Design ®) [2]. Supplementary DSC data were obtained to verify the heat capacity evolution near room temperature. The resulting values are $\Delta_fH°_{298}$(MC) = –8166.4 ± 7.7 kJ/mol and $S°_{298}$(MC) = 652.4 ± 2.2 J/(mol·K). The Gibbs free energy calculated from these values, $\Delta_fG°_{298}$(MC) = −7272.0 ± 8.7 kJ/mol, is in good agreement with solubility measurements [cf. 3].

One major component of Portland cement clinker is Ca_2SiO_4 or C2S (belite) in cement nomenclature. Belite is known to exist in six crystalline polymorphs. The two most common polymorphs are β-Ca_2SiO_4 (larnite) and γ-Ca_2SiO_4 (Ca olivine). Synthetic samples of these phases were investigated by high-temperature oxide melt solution calorimetry in a Calvet type calorimeter at 700 °C [4]; PPMS data were obtained as well.

The results of these measurements yielded so far are:
$\Delta_fH°_{298}$(γ-C_2S) = –2315.1 kJ/mol
$S°_{298}$(γ-C_2S) = 119.7 ± 0.9 J/(mol·K)
$\Delta_fH°_{298}$(β-C_2S) = –2307.7 kJ/mol
$S°_{298}$(β-C_2S) = 123.6 ± 0.9 J/(mol·K)
in good agreement to most literature data [5]. Enthalpy data of Ayed et al. 1994 [6] are not confirmed.

Further experiments on these and other belite polymorphs are in progress.

References

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