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Stability and adhesion of calcite/montmorillonite assembly

W. Sekkal[1], A. Zaoui[1,*] and I. Shahrour[1]

[1]Civil Engineering and geo-Environment Laboratory LGCgE-(EA 4515) Lille Nord de France, Polytech'Lille, Université des Sciences et de la Technologie de Lille, Cité Scientifique, Avenue Paul Langevin, 59655 Villeneuve D'Ascq Cedex, France

Abstract

We analyze here the technical connection between the (104) calcite and (001) montmorillonite surfaces at the atomic level, as well as the conditions to obtain a stable assembly. To this end, the appropriate force field is used to describe the bonding character at the interface. Results show that, in the x direction, the elastic energy provided by calcite to ensure good adhesion at the interface is lower than the one of clay. While in the y direction, it is rather the clay's atoms that provide energy for the accommodation to calcite. Furthermore, we have evaluated, additionally, the adhesion energy, the interfacial distance and the work of separation. We also show that the presence of water molecules at the interface absorb the excess energy and thus contribute to the stabilization of the interface.

Keywords: Clay mineral, adhesion energy, interface, calcite