CORE-LEVEL STUDIES OF CALCITE AND DOLOMITE

by

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Detailed knowledge of chemical bindings on the surface of a mineral is required for theoretical modelling of dissolution processes. For example, Stipp & Hochella (1991) used X-ray photoelectron spectroscopy (XPS) to study bonding environments on the calcite surface. Based on their results, Van Cappellen et al. (1993) created a surface complexation model that postulated the formation of two primary hydration species: $>\text{CO}_3\text{H}^0$ and $>\text{MeOH}^0$, where $>$ represents the mineral lattice and Me is the mineral cation. Our motivation has been to extend the knowledge of chemical bonding on the surfaces of calcite and dolomite.

Both conventional (XPS) and synchrotron-based XPS (SRXPS) were used to record spectra from (104) surfaces of calcite and dolomite that were cleaved in an ultra-high vacuum (UHV) to minimize surface contamination. Surface sensitivity was altered by changing either the measurement angle (XPS) or photon energy (SRXPS). An electron flood gun (Huchital & McKeon 1971) and a conductive mask (Moulder & Hook 1997) were used for charge neutralization.

We discovered that with successful neutralization, it is possible to use SRXPS to obtain peaks that are narrower than the ones obtained with XPS. Narrower peaks enable the elucidation of minor features and acquisition of more accurate results. Surface core-level shifts (SCLS) were found to be between 0.6 and 0.8 eV for Ca 2p (in calcite) and Mg 2p (in dolomite). Some of the satellites in the Ca 2p, C 1s and O 1s spectra of calcite have been interpreted to be bulk plasmons (i.e. collective excitations of electrons) because of their consistency with the density functional theory calculations of Medeiros et al. (2007). A peak in the C 1s spectrum of calcite that is usually attributed to carbide (CaC_2) is suggested to indicate beam-assisted interaction with the hydrocarbons found on the surface.

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