

Revealing and understanding atomic-scale details in the force-field above CaCO_3

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In surface science, the atomic force microscope (AFM) has become an indispensable tool for characterizing surfaces with highest precision. When operated in the non-contact mode (NC-AFM), it allows for measuring forces with the precision of piconewton and with lateral resolution at the scale of single atoms [1]. Calcite, as the most stable polymorph of calcium carbonate CaCO_3 , is of highest interest in various fields, such as biomineralisation. Thus, measuring the force-field above the stable (10.4) cleavage plane is of utmost importance for understanding the interaction of molecules with the surface [2].

We mapped the force field on the (10.4) cleavage plane of calcite in two dimensions by NC-AFM. The data were acquired at room temperature and under ultra-high vacuum (UHV) conditions. The lateral and vertical resolution in the presented dataset is 17 pm and 1 pm, respectively, with a maximum attractive force of around -0.6 nN. We can even differentiate between different carbonate groups within the unit cell [3], which is not possible with standard AFM scanning. Our data match early suggestions by theory, where a relaxation of the carbonate groups towards the tip was proposed [4]. However, simulations giving a more detailed understanding of the atomic-scale mechanisms and, therefore, contrast formation in NC-AFM are still highly desirable.

[1] L. Gross et al., *Science* **325**, 1110 (2009).

[2] P. Rahe et al., *Adv. Mater.* **25**, 25 (2013).

[3] S. Kuhn et al., *submitted*, (2014).

[4] A. Foster et al., *Appl. Surf. Sci.* **188**, 306 (2002).