Experimental Determination of the Adsorption Sites of Individual Metal Atoms on MgO(100) Thin Films

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Magnetic properties of surface-adsorbed atoms are intimately related to the symmetry of the adsorption site. A recent example is given by single Ho atoms adsorbed on MgO(100) thin films grown on Ag(100). These atoms show long magnetic relaxation times due to a ground state that is protected from quantum fluctuations by the symmetry of the adsorption site [1]. For surfaces made of a single element, the adsorption site of adatoms can be determined by means of atomically resolved scanning tunnelling microscopy (STM) images. However, on MgO the atomic protrusions cannot unequivocally be attributed to either of the two atomic species. In addition, the tunnel parameters required for atomic resolution on MgO imply small tip-sample distances where the adatoms are frequently displaced, thus preventing a clear identification of their adsorption site. Hereafter we present a method that solves these issues.

We grow MgO thin films on Ag(100) and use 0.5% doping with Ca, which substitutes Mg. Ca has different STM contrast than Mg and thereby serves as marker for the Mg positions. The adsorption sites of adsorbed Ho atoms, and of any other atom, are determined by extrapolating the MgO lattice from images with atomic resolution of an adsorbate-free surface spot onto an area where the adsorbates are.

After Ho deposition, we observe that two species, with two different apparent heights, coexist on 1 and 2 ML MgO. Using the method described above, we observe that Ho atoms occupy two adsorption sites. They are on-top of O atoms or on bridge sites between two O atoms. We can reversibly switch between these two sites by STM manipulation. In addition, a third Ho species, adsorbed on top of the Mg atom, can be created. This species does not naturally exist upon Ho evaporation and is purely artificial.

Finally we probed the thermal stability of the two species of Ho/MgO that form spontaneously by gently warming up the sample surface up to 50 K. This showed that both species do not diffuse up to this temperature, hence allowing the measurement of the magnetic properties of Ho atoms on a wide range of temperatures.

References

[1] F. Donati, S. Rusponi, S. Stepanow, C. Wäckerlin, A. Singha, L. Persichetti, R. Baltic, K. Diller, F. Patthey, E. Fernandes, J. Dreiser, Ž. Šljivančanin, K. Kummer, C. Nistor, P. Gambardella, H. Brune, Science, **352** (2016) 318.