

Toward Chemical Resolution and Atomic Manipulation with Dynamic AFM

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Using DFT calculations to model the short-range tip-sample interaction we address two key issues in Dynamic AFM: (1) chemical resolution; (2) manipulation of surface atoms using only the chemical tip-sample interaction. The above issues are addressed by a study of an anionic antisite defect on the InP(110) surface. The P atom in the defect and on the perfect InP(110) surface is surrounded by a different "chemical environment". In addition, in the defect there are two possible equilibrium positions of the P atom differing in energy by approx. 0.5 eV. Comparing the simulated AFM images computed for a model Si tip over a perfect surface and defect site provides an estimate of the "chemical identification" capability of the dynamic AFM. The AFM manipulation is simulated by a nanoindentation moving the defect atom with the model tip from one minimum to the other. Manipulations of similar spirit have been reported recently for the Si(111)-7x7 surface [1]. In addition we show that the defect site serves as a convenient initiation point for creation of larger-scale defects, such as removal of P-triplets or even removal of longer In-P chains.

[1] N. Oyabu *et al.*, Phys.Rev.Lett. **90**, 176102 (2003)