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Charging phenomena of supported metal clusters and effects on chemical reactivity: a DFT study

A.A. 2008/2009

Ph.D. dissertation
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first-principles statistical mechanics of lateral interacting adosorbates at metal surfaces

Contents

Acknowledgments

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Cosmin Grigorescu
Eindhoven
February 8, 2010

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Chapter 1

Small Cu islands adsorbed on Ag(100)

nel mezzo del cammin di nostra vita
mi ritrovai per una selva oscura che
la ritta via era smarrita

Dante Alighieri

Abstract

Fast scanning tunneling microscopy reveals an unusual structure and mobility of smaller Cu-islands on clean Ag(100) at room temperature. Whereas islands containing more than 80 atoms exhibit a diffusion and decay behavior similar to the one of homoepitaxed Cu and Ag islands on Cu(100) and Ag(100), respectively, smaller islands show a more complex structure with Cu atoms adsorbed in bridge sites, and a diffusivity and decay time that is significantly higher than any previously measured value. These observations are supported by density-functional theory (DFT) calculations, which indicate a complex reconstructed structure of islands in this size range. Driven by the large lattice mismatch between Ag and Cu, this reconstruction enables shorter Cu-Cu bonds and thereby a stabilization through intra-island strain release. With the concomitantly weakened Cu-Ag bonds, the computed lower binding energy of reconstructed islands to the Ag(100) substrate is consistent with the measured higher diffusivity. In order to arrive at a more quantitative picture we parameterize a three-dimensional Frenkel-Kontorova model with the DFT data, and analyze both the critical island size for reconstruction and the actual diffusion mechanism.

1.1 Introduction

The metal on metal adsorption is a common process in surface science investigations. An important finding in the neurophysiology of the visual system of monkeys and cats, made in the beginning of the 1960s — i.e. before the development of edge detection algorithms for digital image processing — was that the majority of neurons in the primary visual cortex respond to a line or an edge of a certain orientation in a given

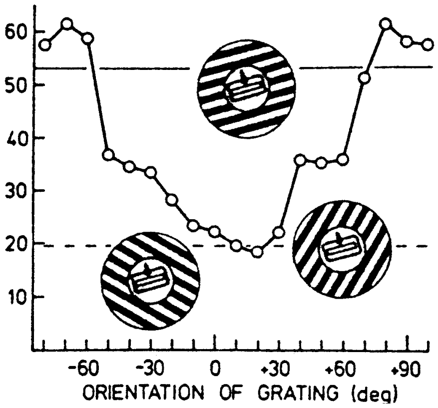

Figure 1.1: *The effect of orientation contrast in non-CRF inhibition: the plot shows the response of a neuron to a stimulus composed of a single bar of optimal orientation in the CRF (central circle) and a grating of varying orientation outside the CRF. The inhibition by the surrounding grating is strongest when its orientation coincides with the optimal stimulus. (Courtesy of C. Blakemore and Exp. Brain Res.).*

position of the visual field. Initially, two types of orientation selective neuron were found, one that was sensitive to the contrast polarity of lines and edges, called simple cell, and another that was not, called complex cell (**?**, **?**).

These computational models gave the basis for biologically motivated edge detection algorithms in image processing. In particular, a family of two dimensional Gabor functions was proposed as a model of the linear filtering properties of simple cells (**?**, **?**).

1.2 Experiments

In the group of Karina Morgenstern (ATOMS, Leibniz University Hannover) a series of STM experiments have been carried out on that system.

Goat 3	Gabor energy	2.0	0.1		0.72	0.38	0.25
	Canny	2.4	0.1		0.83	0.55	0.14
	Anisotropic	2.4	0.1	1.2	0.36	0.60	0.32
	Isotropic	2.0	0.1	1.0	0.46	0.51	0.34
Elephant 2	Gabor energy	2.0	0.1		0.59	0.36	0.32
	Canny	2.4	0.1		0.71	0.50	0.23
	Anisotropic	2.4	0.1	1.2	0.36	0.45	0.40
	Isotropic	2.0	0.1	1.0	0.31	0.49	0.42
Hyena	Gabor energy	2.0	0.1		0.52	0.32	0.39
	Canny	2.2	0.1		0.59	0.50	0.28
	Anisotropic	2.4	0.1	1.2	0.37	0.25	0.51
	Isotropic	2.0	0.1	1.0	0.22	0.35	0.55
Gazelle 2	Gabor energy	2.0	0.1		0.61	0.48	0.32
	Canny	1.6	0.2		0.72	0.38	0.23
	Anisotropic	1.6	0.2	1.0	0.51	0.42	0.36
	Isotropic	1.6	0.2	1.0	0.44	0.46	0.38

Table 1.1: *Operator parameters, errors, and performances for the images presented in Fig.* **??**.