

# Seminář odd. 26

## Tenkých vrstev a nanostruktur

*Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6*

*datum:* 13. 5. 2014 úterý

*čas:* 10:00

*mítnost:* knihovna, budova A, 1.p.

### TÉMA

## STM contrast: The role of the tip

**Krisztian Palotas**

**Budapest University of Technology and Economics,  
Department of Theoretical Physics, Budapest, Hungary**

Understanding scanning tunnelling microscopy (STM) image contrast is of crucial importance in surface science and related technologies. I present different STM tip effects on the contrast in a number of technologically relevant surfaces resulting from first principles calculations. Interestingly, even flat metallic surfaces can show complicated contrast changes depending on the scanning tip and on the tip-sample distance. I show examples for W(110), where orbital-dependent tunnelling [1,2] plays a role, and emphasize the interplay of orbital-dependent tunnelling [1] and spin-polarization effects on constant-current STM images of the Fe(110) surface. Here, the atomic contrast inversion is found to be sensitive to the spin-polarization and the orbital character of the STM tip [3]. Moreover, I present a method to predict the bias-dependent magnetic contrast in surfaces having complex (non-collinear) magnetic order [4]. Finally, taking the highly oriented pyrolytic graphite (HOPG) surface, I demonstrate that the tip orientation has a considerable effect on the simulated STM image contrast [5]. By comparing STM topographic data between experiment [6] and large scale simulations, we can determine particular tip orientations that are most likely present in the STM experiment.

The simulations are performed using the three-dimensional Wentzel-Kramers-Brillouin tunnelling model based on ab initio electronic structure data [7].

#### References:

- [1] K. Palotas et al., Phys. Rev. B 86, 235415 (2012).
- [2] G. Mandi et al., J. Phys.: Condens. Matter 25, 445009 (2013).
- [3] G. Mandi and K. Palotas, Appl. Surf. Sci., accepted (2014) arXiv:1309.4696.
- [4] K. Palotas, Phys. Rev. B 87, 024417 (2013).
- [5] G. Mandi et al., submitted (2014).
- [6] G. Teobaldi et al., Phys. Rev. B 85, 085433 (2012).
- [7] K. Palotas et al., Front. Phys., published online, DOI: 10.1007/s11467-013-0354-4 (2013).

odborný garant: *Ing. Pavel Jelínek, PhD.*