X-ray evidence for mesoscopic relaxations in Cobalt nanoislands on Cu(001)

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Surface x-ray diffraction (SXRD) combined with scanning tunneling microsocopy (STM) and molecular dynamics (MD) calculations gives first evidence that monolayer thick Co nanoislands on Cu(001) experience large relaxations called "mesoscopic misfit " (MM).

The MM was predicted by Stepanyuk at al. [1] several years ago. It was shown that in small Co islands consisting of several tens of atoms only, the average inter-atomic distance is dramatically reduced to values in the 2.40-2.45 Å range as compared to the bulk (2.51 Å). Despite its importance for the physical properties of the islands (e.g. electronic structure and segregation processes [2]) no structural proof for the MM has been provided so far. For instance, STM, x-ray absorption spectroscopy and low energy electron diffraction either do not provide sufficient resolution or must surrender in the case of large ensembles of atoms.

The SXRD analysis is based on the determination of the Co-adlayer registry relative to the Cu(001) surface by probing the intensity distribution along the crystal truncation rods [3]. In contrast to the case of large islands (>>100 atoms), where Co-atoms reside in hollow sites separated by 2.56 Å, Co-atoms in nanoislands also occupy low symmetry sites out of the hollow sites. The experiments were carried out after deposition of sub-monolayer amounts (0.1-0.4 ML) of Co at 170K avoiding intermixing and island coalescence. The MM is identified by giant static disorder of the Co-atoms representing the distribution of adsorption sites around the hollow site position used as equilibrium position for fitting the intensities. On the basis of 8 independent data sets we find a Debye-parameter (B) of the Co-atoms of $B=2.5\pm0.5$ Å^2 (thermal $B\approx0.3$ Å^2). MD calculations using STM images as starting structural models are in excellent agreement with the SXRD derived results.

[1] V. S. Stepanyuk, D.I. Bazhanov, W. Hergert, and J. Kirschner, Phys. Rev. B **63**, 153406 (2001)

[2] M.V. Rastei, B. Heinrich, L. Limot, P.A. Ignatiev, V.S. Stepanyuk, P. Bruno, and J.P. Bucher, Phys. Rev. Lett. **99**, 246102 (2007)

[3] O. Mironets, H. L. Meyerheim, C. Tusche, V.S. Stepanyuk, E. Soyka, P. Zschack, H. Hong, N. Jeutter, R. Felici, and J. Kirschner, Phys. Rev. Lett. **100**, 096103 (2008)