The p4g(2x2) surface reconstruction of magnetic $Fe_4N(100)$

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The compound F_4N is a ferromagnetic material with interesting properties for possible device applications. Thin epitaxial layers of $Fe_4N(100)$ have been grown on Cu(100) substrates in two different UHV set-ups according to a recipe developed in our group [1] whereby Fe is evaporated at a low rate (~100s/Å) in the presence of an atomic nitrogen flow (pressure in the range of 10^{-7}mbar), onto a substrate held at a temperature of ~400ºC. The surface structure and topology of those samples has been studied by combining different techniques: Scanning Electron Microscopy (STM), Low Energy Ion Scattering (LEIS), Auger Electron Spectroscopy (AES) and Low Energy Electron Diffraction (LEED). The experimental results were compared with first principles, ab-initio theoretical calculations.

It is known that bulk Fe_4N has the Fe atoms arranged in an fcc configuration, with the N atoms occupying each fourth octahedral site. Therefore, it is to be expected that the $Fe_4N(100)$ surface has two types of terminations, one with a layer of Fe atoms only and one with a layer containing both Fe and N atoms. However, as we observed the outer layer always contains N.

STM images as well as LEED patterns reveal a non-reconstructed surface (displaying a c(2x2) LEED pattern with respect to Cu(100) and also a p4g(2x2) reconstruction. Some samples show a mixture of these structures, others have only one of them, depending on growth conditions. From LEIS the composition and the structure of two rather pure samples showing either the non-reconstructed structure or the p4g reconstruction were investigated. The atomic positions for Fe and N on the surface were determined by comparing the measured LEIS spectra with simulations carried out with the code MATCH [2]. The experimentally obtained atomic positions agree very well with those predicted by first principles calculations carried out using the SIESTA code. These calculations also show that the average energy of the Fe_4N surface is lowered strongly if N is absorbed in the c(2x2) configuration on an Fe terminated plane with precisely 0.5 monolayer (ML) N coverage. At this coverage the p4g reconstruction is predicted by calculations to occur. The energy gain is less when more, or less, N is absorbed and in these cases the surface will *not* reconstruct. LEED pictures show that the non-reconstructed phase can be converted to p4g by exposing the sample to a flux of atomic N and that the inverse transition can be obtained by evaporating Fe onto the sample surface [3]. Consistent with this observation, AES data show that the nitrogen content in the p4g phase is on average slightly higher than that in the non-reconstructed phase. LEIS measurement probe that the Fe-N ratio in the outer layer was practically equal for the investigated samples.

Based on the experiments and the calculations we propose a model for the phase transition. If excess N is present during the growth at a growth temperature > 300 ºC the coverage with N of the surface will be 0.5 ML and the p4g phase is formed. The excess N is removed by recombination to N_2 molecules. For lower N fluences a non-reconstructed surface or a surface with a mixture of the two structures (due to phase separation) will be formed, depending on the N fluence and possibly on the growth rate.

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