Revisiting the structure of monolayer iron nitride islands on Cu(001)

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Iron nitrides exhibit interesting magnetic and electronic properties, making them promising for applications in spintronics. We studied ultrathin iron nitride islands epitaxially grown on Cu(001) by bombarding the substrate with low-energy N^+ ions, depositing Fe at room temperature and annealing in UHV at 700 K [1]. The geometric parameters of the resulting iron nitride, derived from STM and LEED results, matched those of the "Fe_2N" phase describe in the literature (constituting the middle-plane-cut of the γ'-Fe_4N unit cell). However, the atomic structure exhibited an out-of-plane corrugation not reported by other authors so far. Moreover, XPS revealed a $Fe_{1.3}N$ stoichiometry of the islands, while STS provided a much higher work function value than the one expected for the Fe_2N phase based on DFT calculations. On the basis on these findings, we have developed a new structural model for monolayer iron nitride islands on Cu(001), in which an additional layer of (2×2)-arranged N atoms resides on top of the Fe_2N (resulting in a $Fe_{1.33}N$ stoichiometry) [2]. Notably, LEED-IV calculations confirmed the very good agreement of this model with experimental curves (as judged by the Pendry factor value). We also managed to reduce the islands, via exposure to O_2 at room temperature and UHV annealing, to species with Fe_2N stoichiometry. Thus, direct formation of Fe_2N under specific experimental conditions cannot be excluded.

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