Structure of ultrathin iron films Fcc-to-bcc transitions modified by surfaces

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Iron is bcc and ferromagnetic below 1184 K, but paramagnetic and fcc above this temperature (at zero pressure). Growing thin Fe films on copper appeared to be a straightforward way to stabilize the fcc Fe phase at room temperature. However, beginning in the late 1980s and 1990s it became apparent that ultrathin films grown on copper single crystals exhibit several unusual properties. They are in fact ferromagnetic and show a number of seemingly inexplicable reconstructions. Based on the data available at the time, the most plausible explanation was the assumption of a ferromagnetic fcc phase, also predicted by first principles calculations for heavily strained fcc Fe.

Our STM measurements [1-3] show that the concept of a ferromagnetic fcc phase is neither a useful nor a correct simplification of the crystallography and the energetics of these films. In contrast, all the strong lattice distortions seen in Fe films are variations of the classic martensitic fcc-to-bcc transition. The differences originate in the fact that the phase transitions occur under (1) various constraints by the interface to the substrate and (2) by the presence of the surface. In the case of the Cu(100) substrate, for instance, only films below 5 ML show the fcc-to-nanomartensitic-bcc transformation. Obviously, the lower coordination of the surface atoms and possibly also the substrate-film interface atoms with respect to Fe nearest neighbors plays a crucial role in driving the phase transition in these extremely thin films. Even small clusters fully embedded in Cu like the one in Fig. 1a show these distortions. This suggests that the driving force towards the bcc configuration is much stronger in such isolated arrangements of Fe atoms because of the large interface and surface area relative to the cluster volume.

The most recent results presented in this contribution are:

1) The more or less complete fcc-to-bcc transformation in very small accumulations of Fe atoms (bilayer clusters) and up to 4 ML films on Cu(100) (Fig. 1).

2) The surface reconstruction of 6-8 ML Fe films on Cu(100) (Fig. 2).

3) A new Invar model based on hindered fcc-to-bcc transitions to explain the anomalous thermal expansion of this Fe alloy ($Fe_{65}Ni_{35}$ has near zero thermal expansion between 0 and 500 K) (Fig. 3).

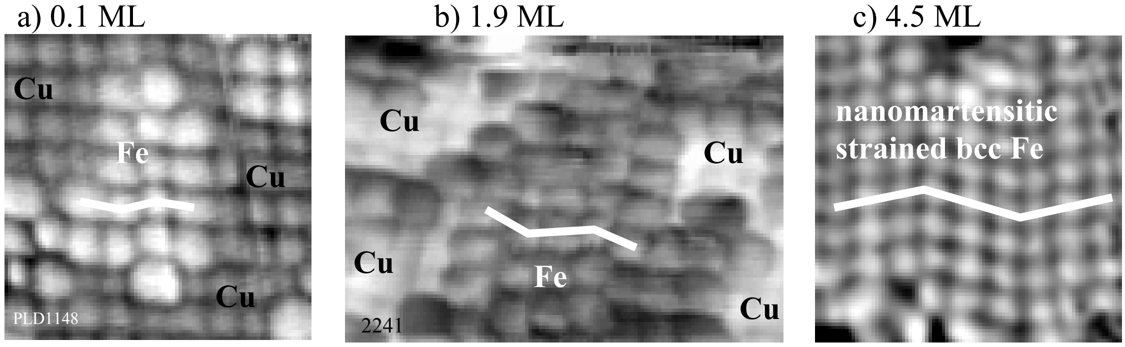

Fig. 1. Ultrathin Fe films on Cu(100). Over the entire thickness range between 0.1 to 4.5 ML clear indications of bcc-like reconstructions are visible, irregular below 2 ML, more regular above 2 ML (white zigzag lines). a) Small embedded Fe clusters at 0.1 ML Fe coverage. Shown is the surface of monolayer islands. It is likely that a few Fe atoms are implanted into the substrate just below the visible surface Fe atoms. b) Nearly closed 2 ML film consisting of Cu and Fe areas of nearly equal size. Note that the image shows inverse atomic corrugation and is therefore rendered with an inverse grayscale. c) 4^{th} ML of a 4.5 ML film.

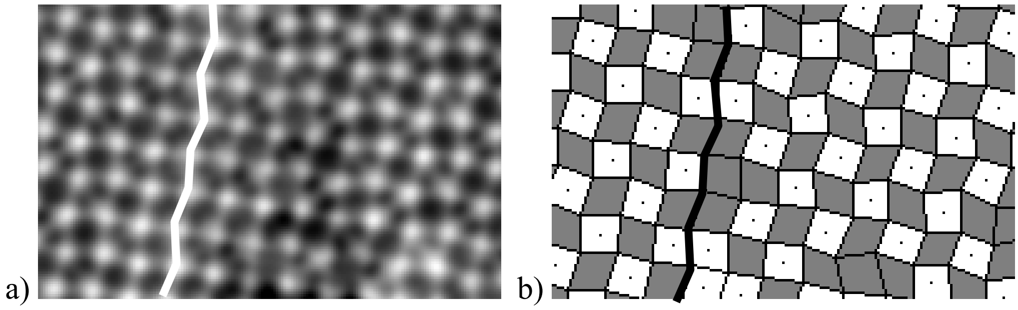

Fig. 2. Surface reconstruction of a 7 ML Fe film grown on Cu(100) at room temperature. a) STM image at 5 K. b) Square-and-rhomb dissection of the STM image characteristic for a p4g(2x2) reconstruction also known as clockwork reconstruction because of the rotated squares. Note the domain boundary crossing the image. The four atoms forming the rhomb configuration and the atom just underneath are almost exactly in the bcc configuration. This suggests that the surface reconstruction is a surface analogon of the bulk fcc-to-bcc transformation.

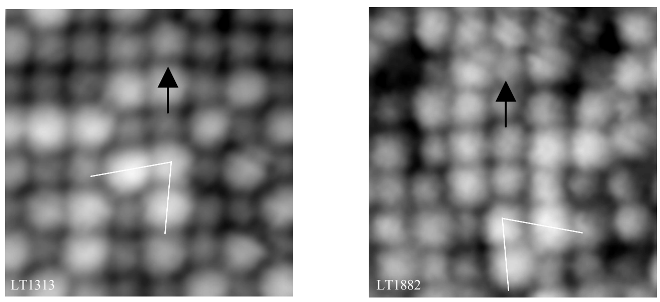

Fig. 3. The (100) surface of an Invar ($Fe_{65}Ni_{35}$) single crystal shows also lattice distortions characteristic for an incomplete fcc-to-bcc transition, though much weaker. In both shown cases, the arrows just above the bright, strongly distorted atom triple indicate a slight in-plane shift (upwards in the image) of a short row of about 3 atoms very similar to the embedded Fe cluster in Fig. 1a. It is likely that such distortions in the bulk of Invar are temperature dependent for the same reasons why Fe is fcc at high temperatures but bcc at low temperatures and cause the vanishing thermal expansion of this alloy.

[1] A. Biedermann, M. Schmid, and P. Varga, PRL 86, 464 (2001).
[2] A. Biedermann, R. Tscheließnig, M. Schmid, and P. Varga, PRL 87, 086103 (2001).
[3] A. Biedermann, R. Tscheließnig, M. Schmid, and P. Varga, Appl. Phys. A 78, 807 (2004).