Erratum: Quantum Size Effect Driven Structure Modifications of Bi Films on Ni(111) [Phys. Rev. Lett. 107, 176102 (2011)]

Tjeerd R. J. Bollmann, Raoul van Gastel, Harold J. W. Zandvliet, and Bene Poelsema

(Received 11 December 2012; published 27 December 2012)

DOI: [10.1103/PhysRevLett.109.269903](https://doi.org/10.1103/PhysRevLett.109.269903)

PACS numbers: 68.55.J-, 68.37.Nq, 73.21.Fg, 99.10.Cd

Inadvertently, we have assigned an incorrect superstructure to the Bi crystallites grown on Ni(111) at 422 K. The selected area diffraction (μ LEED) pattern displayed in Fig. 2(a) represents an (8×8) film structure instead of the assumed (7×7) structure. This implies that the unit cell of the superstructure contains 64 rather than 49 Ni unit cells. With 25 Bi atoms in the supercell we arrive at an increase of the in-plane Bi lattice parameter by $8/7 = 14.3\%$, and thus a reduction of the in-plane density of 23.4%. The recalculated interlayer spacing was not affected, since we derive the interlayer spacing from a tensor-LEED analysis of the I-V dependence of the specular beam, assuming flat and equidistant planes. Therefore, the density of the (8×8) film amounts to 24.90 Bi atoms per nm^3 , i.e., the densities of all three discovered Bi structures, are identical within a few percent. The reduced atomic density leads to an increased Fermi wave length, which now fits 5.0 times in the 7 layer thick film. Table II shows the corrected result. We emphasize that our conclusion remains unaffected: quantum size effects in ultrathin Bi films on Ni(111) are responsible for the observed allotropism.

We gratefully acknowledge Dr. R. M. Tromp, IBM Yorktown Heights, for pointing out the unlikelihood of the large density differences for the three different Bi domains and our incorrect assignment of the “ (7×7) ” structure.

TABLE II. Properties of the three different film structures found: in-plane lattice constant (a_{nn}), film thickness h , interlayer distance derived from tensor-LEED calculation (d_{TL}), density (ρ), fitted number of Fermi wavelengths ($\#\lambda_F$), and corrected calculated deviation from interlayer distance as compared to tensor-LEED calculation.

Structure	(3×3)	$[3-1\ 1\ 2]$	$(8 \times 8)^a$
a_{nn} (Å)	3.73(5)	3.80	3.99
h (# layers)	3	5	7
d_{TL} (Å)	3.21	3.02	2.91
ρ (Bi atoms/ nm^3)	25.79	26.48	24.90
$\#\lambda_F$	2.5	4.0	5.0
$\Delta a_{\text{inter}}/a_{\text{inter}}^b$	4.2%	5.3%	0.2%

^aMeasured at 422 K.^bAssuming that no phase shift occurs at the interfaces.