Erratum: Formation of a well ordered ultrathin aluminum oxide film on icosahedral AlPdMn quasicrystal [Phys. Rev. B 76, 094203 (2007)]

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If the pentagonal surface of the icosahedral AlPdMn quasicrystal is exposed to oxygen, atomically thin oxide domains are formed at the surface involving predominantly Al-O bonds. The lack of Al in the alloy due to this process can adversely affect the stoichiometry and hence the structure of the quasicrystal. In fact, the shift of the concentration towards $Al_{50}(PdMn)_{50}$ results in a known crystalline structure.[3] In this case, the oxide layer is surprisingly similar to that observed on the (110) surface of the ordered NiAl alloy.¹ In order to avoid this formation, oxidation is performed at 700–800 K that promotes segregation of Al from the bulk to the surface and maintains the quasicrystalline stoichiometry. The elevated temperature further promotes the formation of an ordered oxide layer. Similar to the temperature effect, any improper treatment of the surface, *e.g.*, ion bombardment during or after the oxidation process, or improper surface preparation of the quasicrystal prior to oxidation both result in oxide layers typical of those grown on crystalline surfaces.

The model shown in Fig. 3 was proposed as a single domain structure in real-space for the oxide layer on the quasicrystal which was adopted from the oxide structure grown on NiAl(110) (see, *e.g.*, Ref. [22]). In accordance with the global rotational symmetry of the pentagonal surface, there are five degrees of freedom for the rotational alignment of the single domain structure on the pentagonal surface. Consequently, the oxide layer is composed of five distinct twin domains each rotated by multiples of $2\pi/5$ with respect to the others.

Here, we claim that this surface structure is based on unjustified speculations, since (*i*) the twin-domain structure is a consequence of the twofold symmetry of the NiAl(110) surface. The pentagonal surface of *i*-AIPdMn, on the other hand, is fivefold symmetric. (*ii*) The twin-domain model delivers considerably more diffraction spots with the composite pattern than detected in LEED experiments (not shown), and (*iii*) was derived from the LEED pattern shown in Fig. 2c, which was obtained after a brief sputtering of the oxidized surface with Ar^+ ions and subsequent reoxidation. Thus, it represents a surface structure, which most likely differs significantly from the structure shown in Fig. 2b, as mentioned above. Ar^+ ion bombardment was found to shift the structural stability of the quasicrystalline alloy towards the cubic crystal [3,5], therefore, it is not surprising that an oxide layer forms on the sputtered surface which is almost identical to the oxide grown on the (110) surface of the NiAl alloy. The reproduction of the LEED pattern obtained from the Ar^+ ion-bombarded surface using the twin model is very convincing (the reader is referred to Figs. 1c and 1d) and confirms the crystalline interface structure.

¹S. Burkardt and M. Erbudak (unpublished).