Identification of Al Atoms with Different Coordination on Al₂O₃/NiAl(110) Surface with NC-AFM

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In recent years, there have been many reports on the structure of the ultrathin Al_2O_3 film formed on NiAl (110) surface because of its good crystallinity and wide application to heterogeneous catalysis as a stable oxide supports for transition metals and suppression of charging effects as well as fine metal particles on it. Despite the importantance of Al_2O_3 , only little is known about its structure and the proposed structural models of Al_2O_3 are still a debatable issue. In the proposed structural models, Al atoms are bound to O atoms with fourand five-coordination [1]. In the AFM experiments using a metallic Pt-Ir tip, only O atoms are imaged and Al atoms with different coordination are not imaged [2]. Therefore, it is difficult to identify which is a correct structural model.

In this work, we investigate the Al atom imaging with NC-AFM and identify the structural model of the Al_2O_3 on NiAl (110). Because the chemical interaction between the tip and surface plays an important role of AFM imaging, we used the O-terminated Si tip. Si cantilever with the very high stiffness of 2000N/m and very high resonance frequency of 1MHz was used to realize the small amplitude operation, which dominates the short-range interaction force and hence enhances spatial resolution. Figure 1 shows the AFM image with atomic resolution. Al atoms were clearly observed as bright spots, whereas O atoms are observed as dark spots. Interstingly, the four-coordination Al atoms are brighter than the five-coordination Al atoms. As a result, the AFM image is in good agreement with the structural model proposed by DFM calculation [1]. This result with atom selective imaging progresses the research of catalysis by specification of a structural model.



 $5 \text{nm} \times 3.9 \text{nm}$

Fig 1. AFM topography of Al₂O₃ on NiAl (110) and its structural model

- [1] G. Kresse *et al.*, Science **308**, 1440 (2005).
- [2] G. H. Simon et al., New J. Phys. 11, 093009 (2009).