Abstract Submitted
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NC-AFM identification of different aluminum atoms on Al_2O_3/NiAl(110) surface[1] IVAN STICH, JAN BRNDIAR, Inst. of Physics, Slovak Academy of Siences, YAN JUN LI, YASUHIRO SUGAWARA, Dept. of Appl. Phys., Osaka University — Ultrathin alumina film formed by oxidation of NiAl(110) is widely used as a system for technologically important oxide-supported catalysts. Using small amplitude NC-AFM we have obtained images of this system with unprecedented resolution, significantly surpassing the previous STM and NC-AFM images. In particular, we are able to resolve aluminum atoms with different coordination, such as five-, and four-fold coordinated Al atoms. Experiments are supported by extensive density functional theory modeling. Starting from the previous atomic model [1], we have been able to describe the gross image features such as the dark oxygen sites. We find that the system is strongly ionic with the oxygen sites strongly negatively charged and aluminum sites positively charged. Hence, the NC-AFM images can reliably be understood from electrostatic potentials. These finding also suggest an oxygen terminated apex. Resolving finer contrast features of the differently coordinated Al atoms required construction of better and more realistic approximants to the ultra-thin incommensurable alumina interface. [1] G. Kresse et al., Science **308**, 1440 (2005).

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