Surface reconstruction of the polar spinel $MgAl_2O_4(001)$

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The detailed surface structure is key to understanding the surface chemistry of materials. Magnesium aluminate ($MgAl_2O_4$, spinel), which gave the group of spinel minerals its name, is a wide-gap insulator and poses considerable challenges for experimental surface characterization. In this work, noncontact atomic force microscopy (nc-AFM) with a qPlus sensor [1] and a controlled tip apex [2] was used to resolve the atomic-level surface structure. The $MgAl_2O_4(001)$ surface adopts a c(2 × 4) reconstruction accompanied by a modification of surface stoichiometry. The reconstructed surface is enriched in aluminum and contains ordered pairs of octahedrally coordinated magnesium atoms replacing their tetrahedral bulk sites. This charge redistribution within the reconstructed surface layer stabilizes the otherwise polar $MgAl_2O_4(001)$ termination. The proposed surface reconstruction closely resembles those found on other spinel oxides, such as $Fe_3O_4(001)$ [3] and $Mn_3O_4(001)$ [4], suggesting a universal mechanism for compensating the polarity of spinel surfaces.

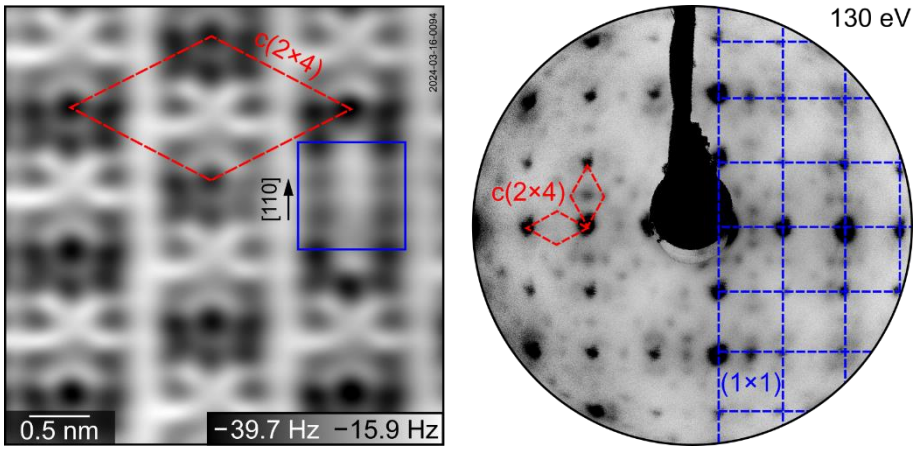

Figure 1: The reconstructed $MgAl_2O_4(001)$ surface. (a) Nc-AFM image acquired with a CuOx terminated tip. The unit cell of the c(2 × 4) reconstructed surface is indicated by a red dashed rhombus, a locally unreconstructed area is surrounded by a blue rectangle. (b) LEED pattern of the reconstructed surface. The blue dashed grid indicates the bulk (1 × 1) reciprocal lattice, the two red rhombi highlight the c(2 × 4) and c(4 × 2) cells.

References

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