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FROM A SINGLE IMAGE TO A 3D SHAPE OF A NANO-SCALE MgO CRYSTAL WITH ATOMIC RESOLUTIION

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Abstract

The accurate description of the physical and chemical properties of nanoscale materials is a long-standing goal in nanoscience and technology. Many of the interesting properties of such dimensionally limited systems result from the dominant part played by their surface structure and chemistry, which are related intimately to their functionality [1]. An important example is the use of nanoparticles in catalysis, where the chemical reactivity depends on both the atomic species and the particular atom arrangement present on the surface [2].

Although the overall atomic structure of a nanoscale crystal is in principle accessible by modern transmission electron microscopy, the precise determination of its surface structure is an intricate problem. In the present work, we show that aberration-corrected transmission electron microscopy, combined with dedicated numerical evaluation procedures, allows the three-dimensional shape of a thin MgO crystal to be determined from only one single high-resolution image [3]. The sensitivity of the reconstruction procedure is not only sufficient to reveal the surface morphology of the crystal with atomic resolution, but also to detect the presence of adsorbed impurity atoms. Our single-image approach can be highly advantageous, or may indeed be the only alternative, when dealing with radiation-sensitive crystals, for which it is often impossible to acquire more than a single image before the atomic structure has changed. The possibility to detect changes in surface morphology during *in situ* chemical reactions is also now within reach due to the advantage of using a very short acquisition time. The present single-image approach therefore offers broad application potential for atomically resolved 3D studies of nanoscale crystalline materials.

References

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