FIRST CROSS-SECTIONAL ANALYSIS OF MgO {100} SURFACES BY C_s-CORRECTED TEM. Jun Yamasaki(1), Nobuo Tanaka(1), Yoshihiro Nakagaki(2), Syunsuke Fukami(2), and Hidetaka Sawada(3). (1)EcoTopia Science Institute, Nagoya University, Nagoya, 464-8603, Japan; (2)Department of Crystalline Materials Science, Nagoya University, Nagoya, 464-8603, Japan; (3)JEOL Ltd., Akishima, Tokyo, 196-8558 Japan.
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Recently, a spherical-aberration (C_s) corrected 200kV TEM has brought a significant improvement in its spatial resolution, which allows us to identify even oxygen atom columns in crystalline materials [1, 2]. Another important advantage of C_s-correction is that non-periodic structures such as surfaces/interfaces and tubes are observed precisely at almost just focus [3, 4, 5]. In the present study we have succeeded in analyzing surface structures of MgO {100} by a C_s-corrected TEM.

We used a 200kV TEM (JEOL:JEM-2100F) equipped with a C_s-corrector [6]. MgO crystalline thin films for TEM observations were prepared by electron-gun evaporation onto NaCl substrates in vacuum of 5 x 10^{-8} Pa. After removal of the substrates by water, the MgO films were mounted on micro-grids. Pinholes of several nm diameter were created in the films in a TEM (1x10^{-5}Pa) by a focused electron probe (Figure 1). We observed clean {100} surfaces on the sidewalls of the pinholes cross-sectionally (Figure 2). The Mg and O atom columns appear as larger and smaller dark dots in the perfect crystal area that lies underneath the {100} surface layer. On the other hand, dark and bright contrasts in the surface layer elongate toward vacuum as indicated by black and white arrows in the figure, respectively. It has been known that there is no remarkable reconstruction on clean {100} surfaces of MgO except for slight rumpling and relaxation [7]. Image simulations based on such slight structural changes do not, however, reproduce the elongation of the contrasts in Figure 2 at any values of defocus and thickness (Figure 3a). It is considered that the elongation is related to surface adatoms/vacancies of Mg or O atoms created during the vaporization of the MgO films by the focused electron probe. We have estimated structural changes induced by the surface point defects roughly by Madelung energies. The result indicates that a pair of vacancies at a sub-lattice, such as V_{Mg}-V_{Mg} and V_O-V_O, induces displacement of adjacent atoms at another sub-lattice about 0.1 nm toward vacuum. Image simulations of the structure model in which some vacancies are introduced randomly on a MgO {100} surface reproduce the elongation of the contrasts in Figure 2 (Figure 3b). It is considered that we have succeeded for the first time in observing structural changes induced by surface lattice defects on MgO{100}.

It is difficult to detect this kind of local structural changes by using diffraction or spectroscopic methods and an ordinary TEM. Images with a non-zero C_s value do not give us intuitive predicts of surface structures as shown in Figure 3c owing to lack of spatial resolution and artificial contrast near the surfaces by significant defocus values. It is considered that Cs-corrected TEMs make it possible to analyze surface structures with a high degree of accuracy.

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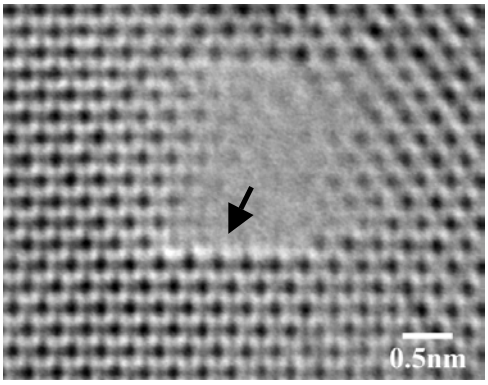

Figure 1. Pinhole created in a MgO{110} thin film by a focused electron probe in a TEM. Clean {100} surfaces are formed at edges of the pinhole (see an arrow).

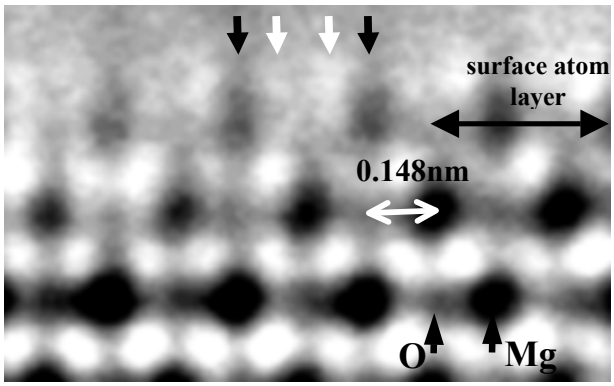

Figure 2. Actual cross-sectional observation of the clean MgO{100} surface under Cs = 0. Dark and bright contrasts in the surface atom layer elongate toward vacuum as indicated by black and white arrows.

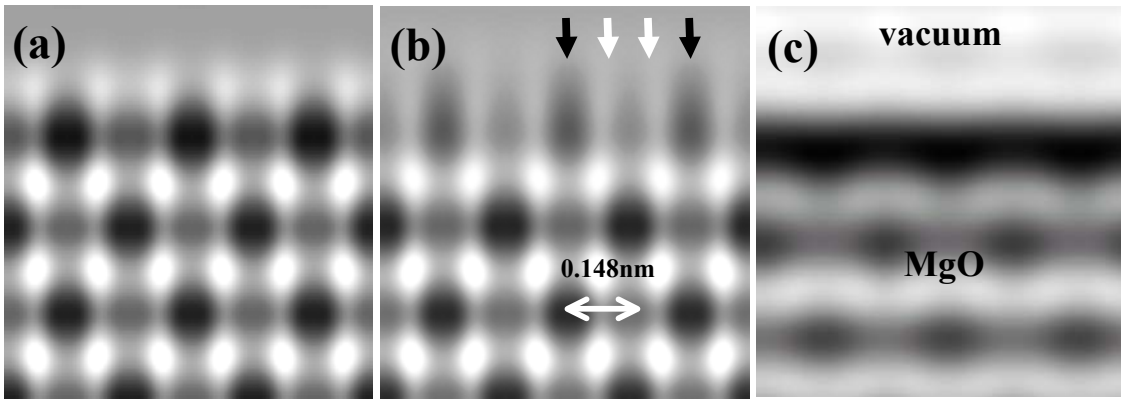

Figure 3. Image simulations of MgO{100} surfaces. (a) Surface without reconstruction (C_s = 0). (b) Reconstructed surface induced by surface vacancies. The elongation of the contrasts in Figure 2 is reproduced (C_s = 0). (c) Surface without reconstruction observed by an ordinary 200 kV TEM (C_s = 0.5 mm).