Electron beam-assisted healing of nanopores in magnesium alloys

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Supplementary Material Includes:

Figures S1-S5

Table S1

Movies S1-S3

Discussion

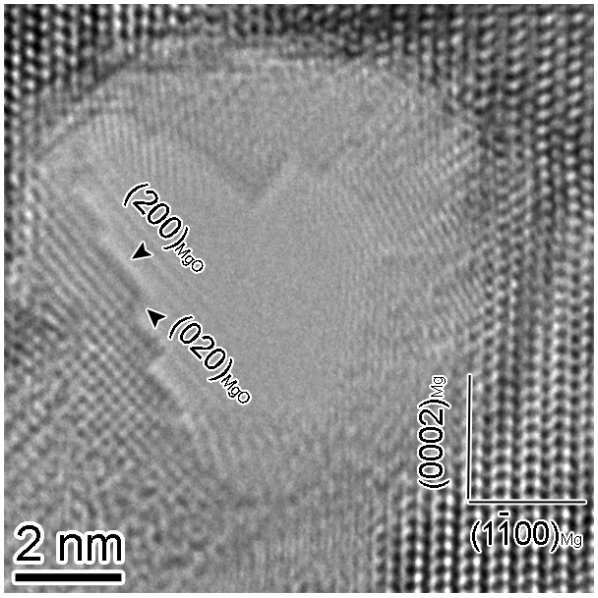

Figure S1. Oxidation of nanopore periphery. A typical HRTEM image showing that the nanopore sidewalls were oxidized as a result of 30-minute e-beam irradiation. The surface steps pointed out by the arrow heads are enclosed by (200) and (020) planes of the cubic MgO phase, similar to that observed in Figs. 2h and 2i.

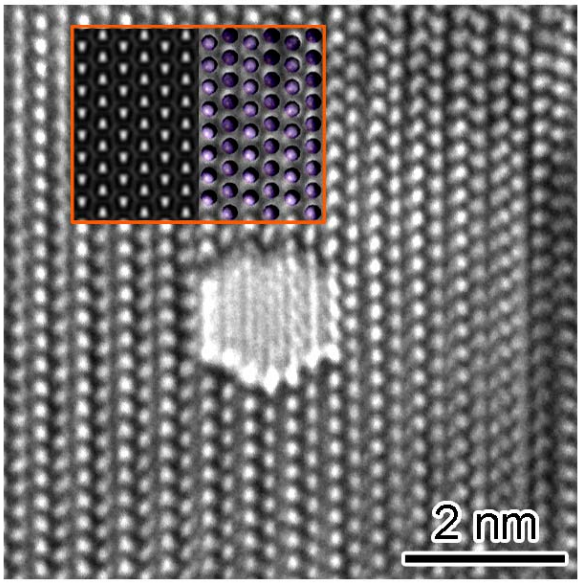

Figure S2. The typical HRTEM image shown in Fig. 3f. The inset shows a simulated HRTEM image and a related atomic model, consistent with the experimental observation. Based upon the simulation results, the sample thickness was estimated to be 10 nm. The white dots in the images correspond to the actual atomic columns of Mg. The simulations were conducted by applying the parameters including an acceleration voltage of 200 kV, a spherical aberration coefficient of 0.5 mm, and a focus value of -49 nm.

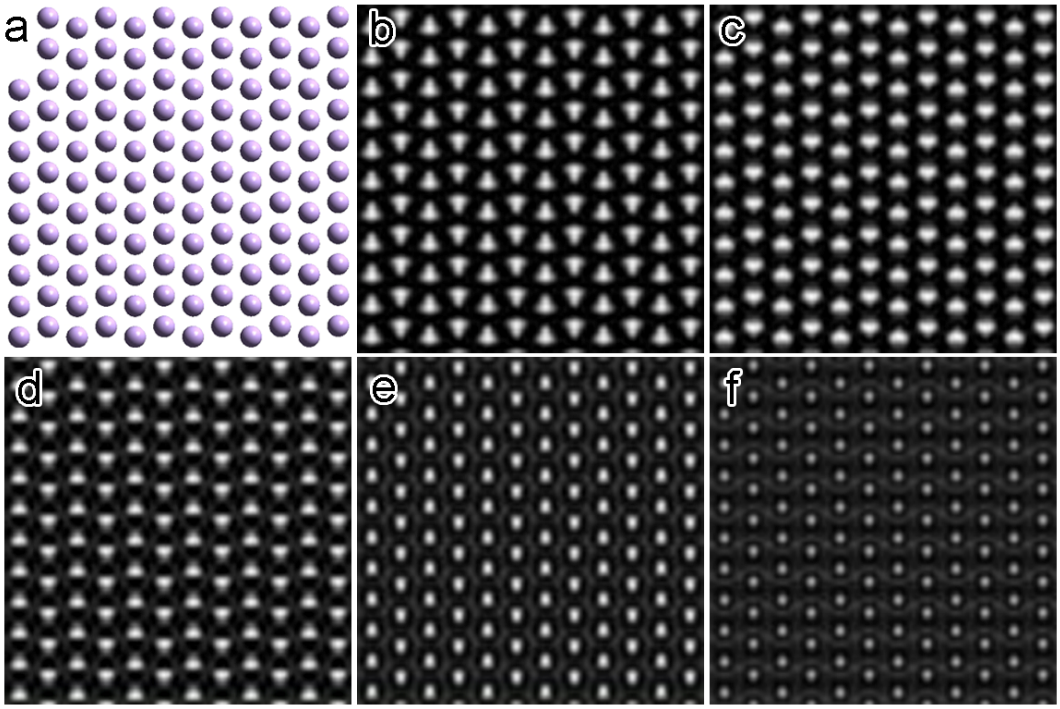

Figure S3. Image simulation of a Mg crystal along the [11$\bar{2}$0] zone axis applying the parameters including an acceleration voltage of 200 kV, a spherical aberration coefficient of 0.5 mm. (a) The corresponding structural model of Mg. (b-f) The simulated images with sample thickness of 10 nm and focus values of -61, -57, -53, -49, and -45 nm, respectively.

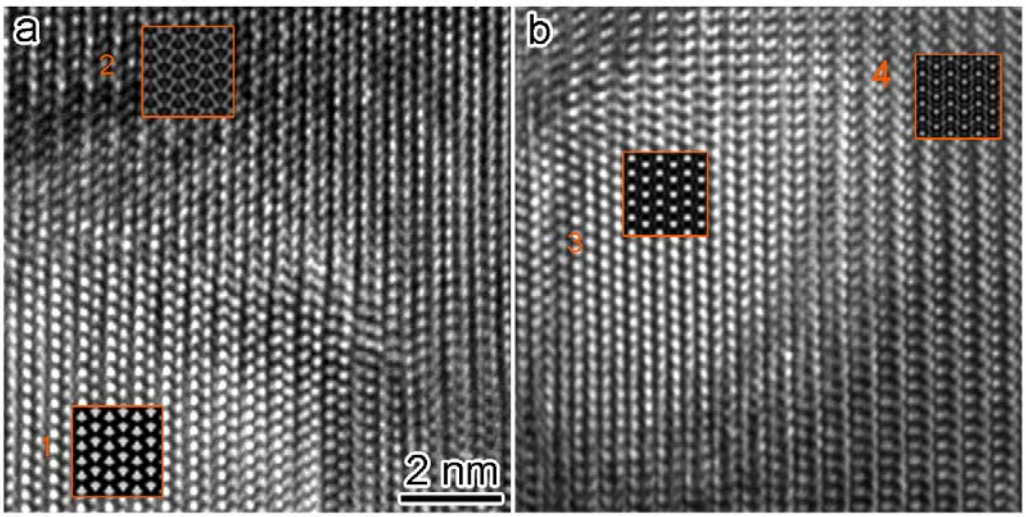

Figure S4. Estimation of the sample thickness. **(**a-b) Two typical HRTEM images after two individual nanopores healed. Evidently, the healed regions (1 and 3) show the brighter contrast as compared with the rest part of the sample (2 and 4). The insets show the simulated HRTEM images, which are consistent with the experimental observation. Based upon the simulation results, the sample thicknesses in regions 1 to 4 were

estimated to be 9, 27, 9, and 14 nm, respectively. The simulations were conducted by applying the parameters including an acceleration voltage of 200 kV, a spherical aberration coefficient of 0.5 mm and the focus values of -60 nm in regions 1 and 2, and -15 nm in regions 3 and 4. The healed nanopore in (b) corresponds to that shown in Fig. 2f.

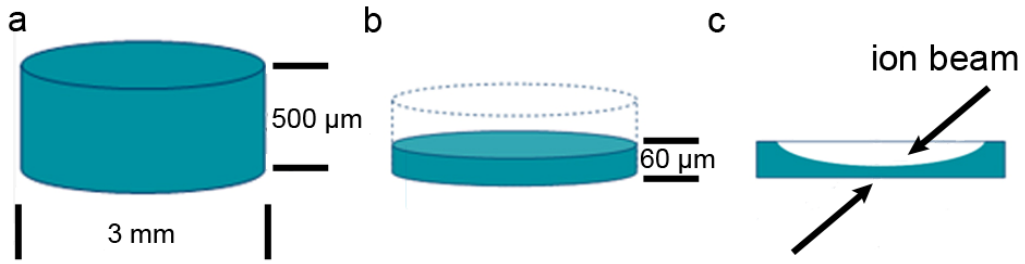

Figure S5. Schematic depiction of the TEM sample preparation process.

Table S1 The d_1/d_i (i=2-4) values calculated at the moment before the nucleation of a new {0002} layer concerning 34 growth events. The values less than 1 are presented by the red fonts. The initial size of four nanopores represented by "A", "B", "C", and "D" is 4.5, 4.4, 3.3, and 3.4 nm, respectively. The related subscripts indicate the nucleation events.

d_1/d_i	d_1/d_2	d_1/d_3	d_1/d_4
A_1	1.43	1.44	1.38
A_2	1.46	1.37	1.31
A_3	1.28	1.30	1.23
A_4	1.20	1.22	1.14
A_5	1.22	1.23	1.14
A_6	1.23	1.13	1.15
A_7	1.14	1.04	1.18
A_8	1.04	1.18	1.20
A_9	1.07	1.09	1.12
A_{10}	0.98	0.99	1.00
A_{11}	1.12	1.13	1.01
B_1	1.09	1.09	1.13
B_2	1.09	1.21	1.15
B_3	1.09	1.14	1.14
B_4	1.15	1.07	1.08
B_5	1.15	0.99	1.00
B_6	1.05	1.06	1.18
B_7	1.12	1.06	1.08
B_8	1.08	1.06	1.20
B_9	1.21	1.22	1.20
B_{10}	1.06	1.07	1.05
B_{11}	1.04	1.06	1.19
C_1	0.94	0.94	0.98
C_2	1.24	1.32	1.18

C_3	1.02	1.09	0.98
C_4	1.22	1.14	1.13
C_4	0.87	0.94	1.09
D_1	1.32	1.01	1.06
D_2	1.21	1.02	1.07
D_3	1.13	0.94	1.08
D_4	1.45	1.05	1.08
D_5	1.30	0.94	0.98
D_6	1.34	1.07	1.26
D_7	1.40	1.10	1.29

Movie S1: The dynamic evolution of the healing process of a nanopore with an original size of 3.3 nm, played at 5× speed (2 frames/sec).

Movie S2: Layer-by-layer growth of lattice planes at the nanopore periphery, played at 30× speed (2 frames/sec).

Movie S3: Anisotropic atomic diffusion during the healing process, played at 20× speed (2 frames/sec).

Supplementary Discussion

1. HRTEM simulations

The simulated HRTEM image and correlated structural model (inset in Fig. S2) reveal that the white dots in Fig. 3f represent the actual atomic columns of Mg. The sample thickness (*t*) around the nanopore and focus value (*d*) were estimated to be 10 nm and -49 nm, respectively. Furthermore, the simulated images with *d* ranging from -61 to -45 nm and *t*=10 nm are presented in Figs. S3b-S3f. Because *d* will not change significantly during the experiment (Figs. 3a-3f), it is believed that the white dots shown in Figs. 3a-3f consistently stand for the actual atomic columns of Mg, as illustrated by the corresponding structural models shown in Figs. 3g-3l.

2. Error analysis

The nanopore width here was obtained by measuring several times and then getting the averaged value, which may suffer from an error of less than 5%.