High temperature mediated rocksalt to wurtzite phase transformation in cadmium oxide nano-sheets and their theoretical evidences

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Table 1S: Inter-planner spacing values from XRD pattern

| Sample name | Particle diameter (nm) | 2θ position | Plane | Inter-planner spacing |
|-------------|------------------------|-------------|-------|-----------------------|
| CdO500      | 27                     | 33.1        | (101) | 2.70 Å                |
|             | 38.4                   | (200)       |       | 2.34 Å                |
|             | 55.4                   | (220)       |       | 1.66 Å                |
| CdO700      | 30                     | 33.1        | (101) | 2.70 Å                |
|             | 38.4                   | (200)       |       | 2.34 Å                |
|             | 55.4                   | (220)       |       | 1.66 Å                |
| CdO900      | n.a.                   | 37.1        | (101) | 2.42 Å                |
|             | 48.6                   | (102)       |       | 1.87 Å                |
Figure 1S: Rietveld refinement for CdO500, CdO700, CdO900 thin films are shown at (a), (b), (c) respectively
Table 2S: Rietveld refined parameters for various compositions in the system

(a) Results of the Rietveld refinement for CdO500

| Ions  | x     | y     | z     | B<sub>iso</sub> (Å<sup>2</sup>) |
|-------|-------|-------|-------|-------------------------------|
| Cd<sup>2+</sup> | 0     | 0     | 0     | 1.002                         |
| O<sup>2-</sup>  | 0.5   | 0.5   | 0.5   | 1.075                         |

R-factors: \(R_p = 14.2, R_{wp} = 19.7, R_{exp} = 16.95, \chi^2 = 1.35\)

(b) Results of the Rietveld refinement for CdO700

| Ions  | x     | y     | z     | B<sub>iso</sub> (Å<sup>2</sup>) |
|-------|-------|-------|-------|-------------------------------|
| Cd<sup>2+</sup> | 0     | 0     | 0     | 1.450                         |
| O<sup>2-</sup>  | 0.5   | 0.5   | 0.5   | 0.512                         |

R-factors: \(R_p = 17.6, R_{wp} = 22.8, R_{exp} = 21.18, \chi^2 = 1.16\)

(c) Results of the Rietveld refinement for CdO900

| Ions  | x     | y     | z     | B<sub>iso</sub> (Å<sup>2</sup>) |
|-------|-------|-------|-------|-------------------------------|
| Cd<sup>2+</sup> (I) | 0.33330 | 0.66670 | 0.99960 | 1.100                        |
| Cd<sup>2+</sup> (II) | 0.66670 | 0.33330 | 0.49960 | 1.100                        |
| O<sup>2-</sup> (I)  | 0.33330 | 0.66670 | 0.38530 | 0.886                        |
| O<sup>2-</sup> (II) | 0.66670 | 0.33330 | 0.88530 | 0.886                        |

R-factors: \(R_p = 24.5, R_{wp} = 31.9, R_{exp} = 25.43, \chi^2 = 1.57\)
Table 3S: Fitting parameters for O 1s and Cd 3d XPS spectra

|                          | peak position | peak FWHM | peak area | CdO$_500$ 2nd etching peak position | peak FWHM | peak area | CdO$_500$ 4th etching peak position | peak FWHM | peak area |
|--------------------------|---------------|-----------|-----------|-------------------------------------|-----------|----------|-------------------------------------|-----------|----------|
| Cd(OH)$_2$/CdCO$_3$      | 532.07        | 1.74      | 12285     | 531.7                               | 2.05      | 5497     | 531.4                               | 2.1       | 5540     |
| CdO                      | 528.9         | 1.12      | 1930      | 529.0                               | 0.86      | 6555     | 529.1                               | 0.96      | 9903     |
| CdO$_2$                  | 529.6         | 0.87      | 310.9     | 529.6                               | 1.28      | 4707     | 529.7                               | 0.77      | 1497     |
| Cd(OH)$_2$/CdCO$_3$      | 532.08        | 1.76      | 12105     | 531.2                               | 2.61      | 8196     | 531.1                               | 3.22      | 12902    |
| CdO                      | 528.9         | 1.12      | 1940      | 529.8                               | 0.91      | 1498     | 529.7                               | 0.58      | 656      |
| CdO$_2$                  | 529.6         | 0.88      | 299       | 529.6                               | 1.06      | 1498     | 529.7                               | 0.58      | 656      |
| Cd(OH)$_2$/CdCO$_3$      | 531.8         | 1.45      | 8509      | 531.7                               | 1.44      | 8303     | 531.8                               | 1.40      | 8106     |
| CdO                      | 530.1         | 1.57      | 16502     | 530.1                               | 1.56      | 17301    | 530.2                               | 1.59      | 18782    |
| CdO$_2$                  | n.a.          | n.a.      | n.a.      | n.a.                                | n.a.      | n.a.     | n.a.                                | n.a.      | n.a.     |
| Cd(OH)$_2$/CdCO$_3$      | 404.2         | 1.19      | 14519     | 404.4                               | 1.0       | 51130    | 404.4                               | 1.04      | 52390    |
| CdO                      | 405.2         | 1.21      | 6296      | 405.3                               | 1.6       | 39863    | 405.3                               | 1.6       | 43184    |
| CdO$_2$                  | 405.9         | 1.22      | 19820     | n.a.                                | n.a.      | n.a.     | n.a.                                | n.a.      | n.a.     |
| Cd(OH)$_2$/CdCO$_3$      | 405.9         | 1.22      | 19820     | n.a.                                | n.a.      | n.a.     | n.a.                                | n.a.      | n.a.     |
| CdO                      | 404.5         | 1.19      | 14519     | 404.4                               | 1.07      | 50265    | 404.4                               | 1.38      | 46065    |
| CdO$_2$                  | 405.5         | 1.21      | 6296      | 405.3                               | 1.6       | 43076    | 405.5                               | 1.37      | 33030    |
| CdCO$_3$/Cd(OH)$_2$      | 406.2         | 1.22      | 19820     | n.a.                                | n.a.      | n.a.     | n.a.                                | n.a.      | n.a.     |
| CdO                      | 405.5         | 1.21      | 6296      | 405.3                               | 1.6       | 43076    | 405.5                               | 1.37      | 33030    |
| CdO$_2$                  | 405.5         | 1.22      | 19820     | n.a.                                | n.a.      | n.a.     | n.a.                                | n.a.      | n.a.     |
Figure 2S: Depth profiling for CdO500, CdO700, CdO900 thin films
Figure 3S: Section analysis of CdO500, CdO700, CdO900 thin films with nanoscope software
Figure 4S: Schematic illustration of nanosheet formation