Electronic Supplementary Material (ESI) for Nanoscale.

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

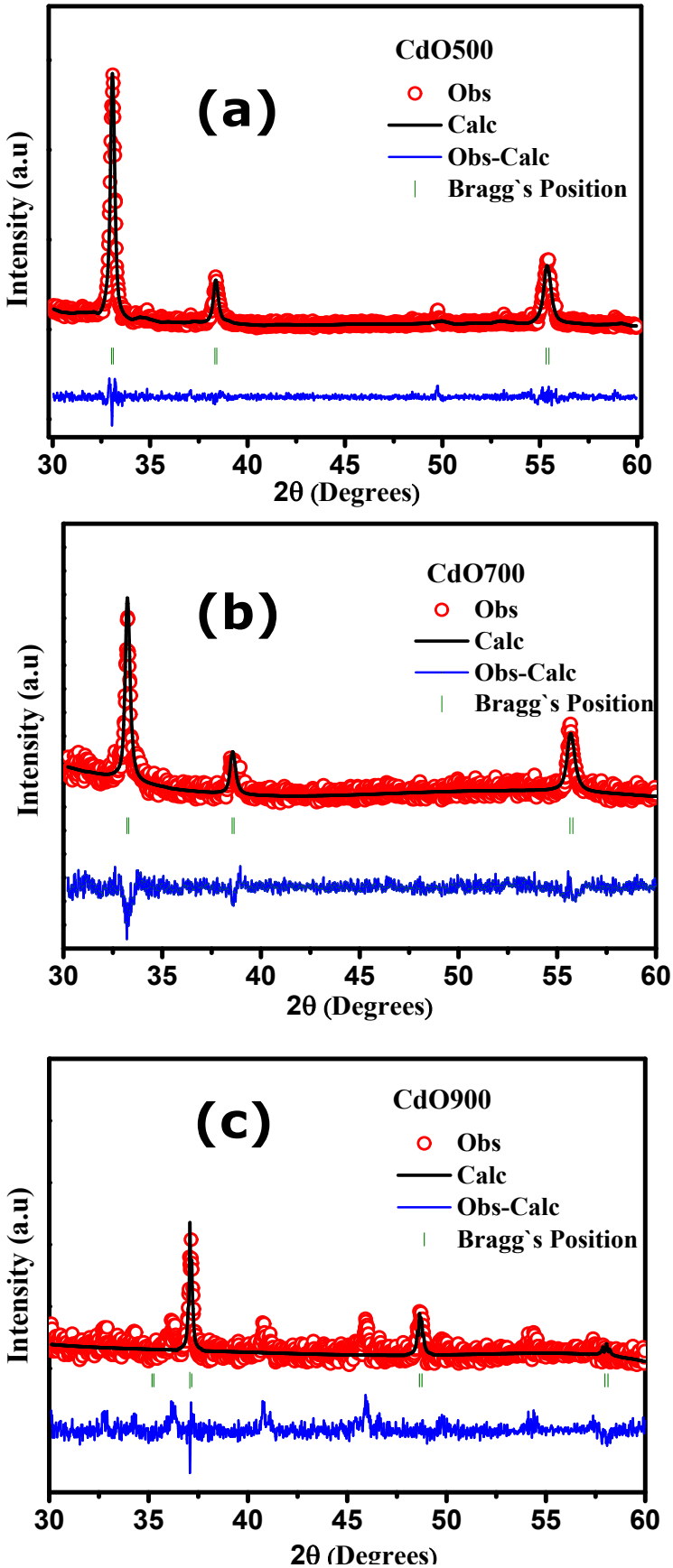

Figure 1S: Rietveld refinement for CdO500, CdO700, CdO900 thin films are shown at (a), (b), (c) respectively

Table 2S: Rietveld refined parameters for various compositions in the system

(a) Results of the Rietveld refinement for CdO500

Cubic phase with space group *Fm-3m* a = b = c = 4.69342 (15) Å, α = β = γ = 90°				
Ions	*x*	*y*	*z*	B_{iso} (Å^2)
Cd^{2+}	0	0	0	1.002
O^{2-}	0.5	0.5	0.5	1.075
R-factors	R_p = 14.2, $R_{w\text{-}p}$ = 19.7, R_{exp} = 16.95, χ^2 = 1.35			

(b) Results of the Rietveld refinement for CdO700

Cubic phase with space group *Fm-3m* a = b = c = 4.69342 (15) Å, α = β = γ = 90°				
Ions	*x*	*y*	*z*	B_{iso} (Å^2)
Cd^{2+}	0	0	0	1.450
O^{2-}	0.5	0.5	0.5	0.512
R-factors	R_p = 17.6, $R_{w\text{-}p}$ = 22.8, R_{exp} = 21.18, χ^2 = 1.16			

(c) Results of the Rietveld refinement for CdO900

Hexagonal phase with space group P 63 m c a = b = 3.18594 (9) Å, c = 5.10303 (7) Å, α = β = 90°, γ = 120°				
Ions	*x*	*y*	*z*	B_{iso} (Å^2)
Cd^{2+} (I)	0.33330	0.66670	0.99960	1.100
Cd^{2+} (II)	0.66670	0.33330	0.49960	1.100
O^{2-} (I)	0.33330	0.66670	0.38530	0.886
O^{2-} (II)	0.66670	0.33330	0.88530	0.886
R-factors	R_p = 24.5, $R_{w\text{-}p}$ = 31.9, R_{exp} = 25.43, χ^2 =1.57			

Table 3S: Fitting parameters for O 1s and Cd 3d XPS spectra

On surface CdO500 (O 1s)	peak position	peak FWHM	peak area	CdO500 2nd etching peak position	peak FWHM	peak area	CdO500 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
On surface CdO700 (O 1s)	peak position	peak FWHM	peak area	CdO700 2nd etching peak position	peak FWHM	peak area	CdO700 4th etching peak position	peak FWHM	peak area
$Cd(OH)_2$/ $CdCO_3$	532.08	1.76	12105	531.2	2.61	8196	531	3.22	12902
CdO	528.9	1.12	1940	529	0.88	7707	529.1	0.82	6240
CdO_2	529.6	0.88	299	529.8	0.91	1498	529.7	0.58	656
On surface CdO900 (O 1s)	peak position	peak FWHM	peak area	CdO900 2nd etching peak position	peak FWHM	peak area	CdO900 4th etching peak position	peak FWHM	peak area
$Cd(OH)_2$/ $CdCO_3$	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.
On surface CdO500 (Cd 3d)	peak position	peak FWHM	peak area	CdO500 2nd etching peak position	peak FWHM	peak area	CdO500 4th etching peak position	peak FWHM	peak area
CdO	404.2	1.19	14519	404.4	1.0	51130	404.4	1.04	52390
CdO_2	405.2	1.21	6296	405.3	1.6	39863	405.3	1.6	43184
$CdCO_3$/ $Cd(OH)_2$	405.9	1.22	19820	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
On surface CdO700 (Cd 3d)	peak position	peak FWHM	peak area	CdO700 2nd etching peak position	peak FWHM	peak area	CdO700 4th etching peak position	peak FWHM	peak area
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.
On surface	peak position	peak FWHM	peak area	CdO900 2nd	peak FWHM	peak area	CdO900 4th	peak FWHM	peak area

CdO900 (Cd 3d)				etching peak position			etching peak position		
CdO	405.3	1.21	21319	404.8	1.40	63008	404.9	1.41	66314
$CdCO_3$/ $Cd(OH)_2$	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

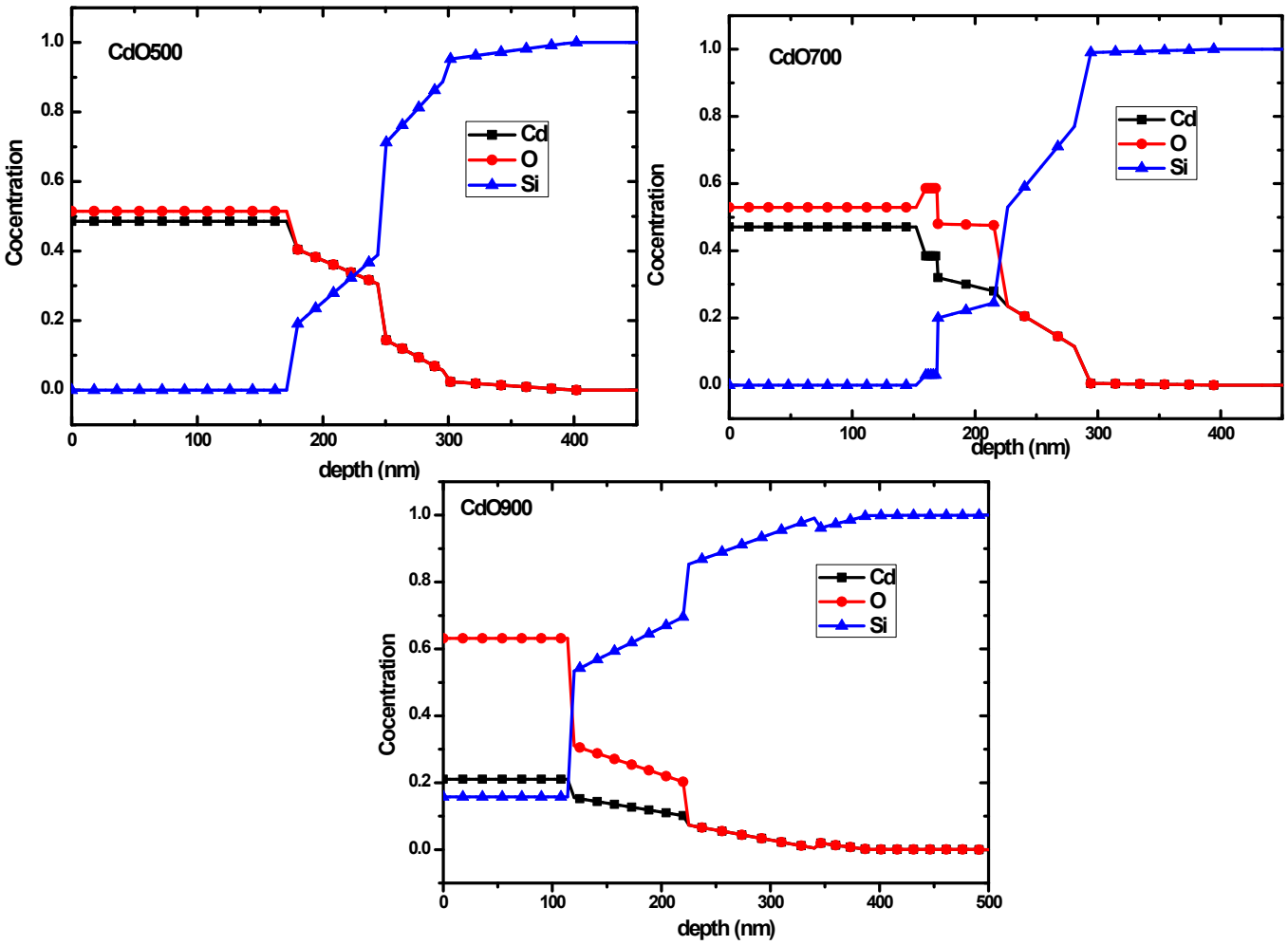

Figure 2S: Depth profiling for CdO500, CdO700, CdO900 thin films

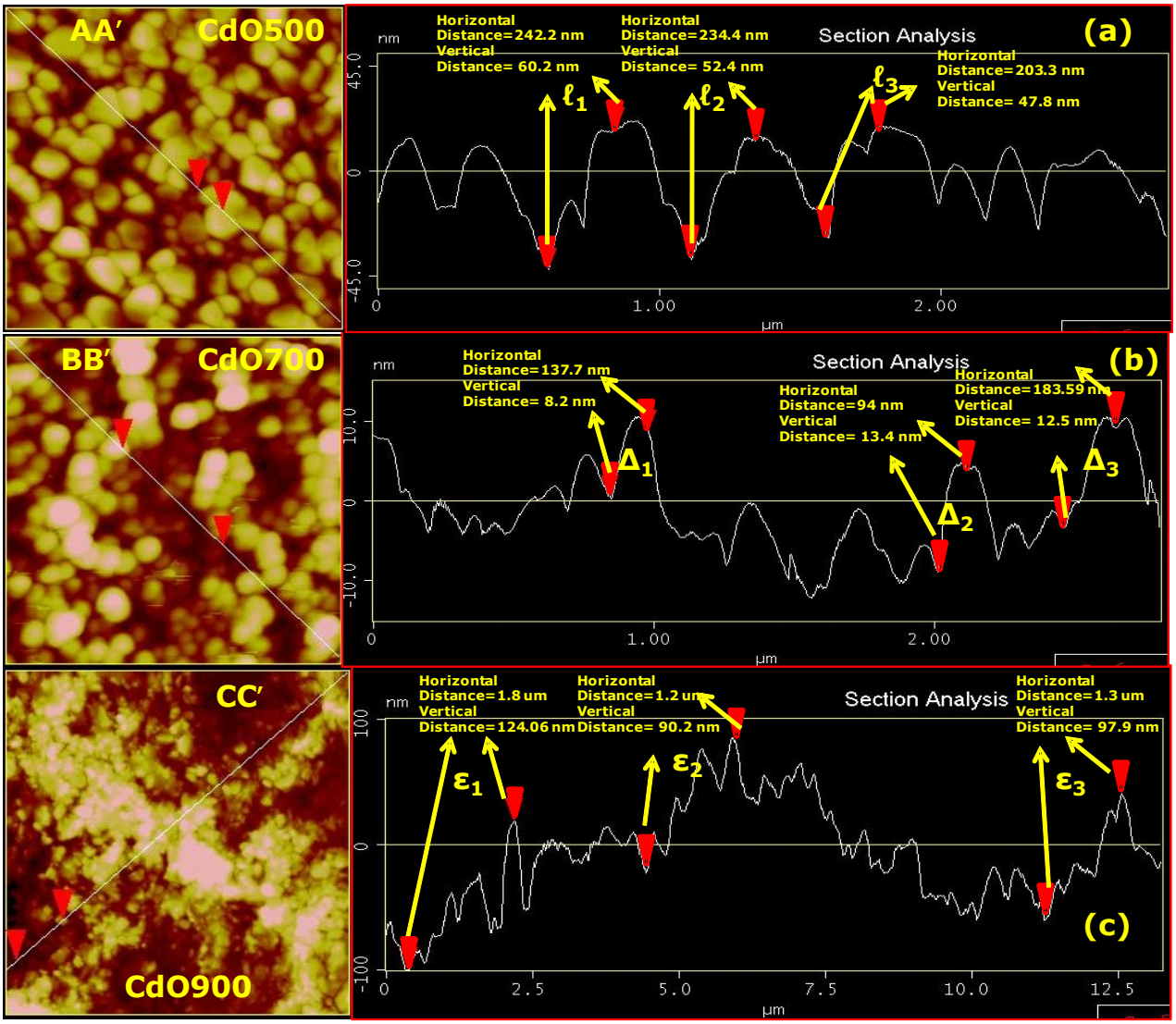

Figure 3S: Section analysis of CdO500, CdO700, CdO900 thin films with nanoscope software

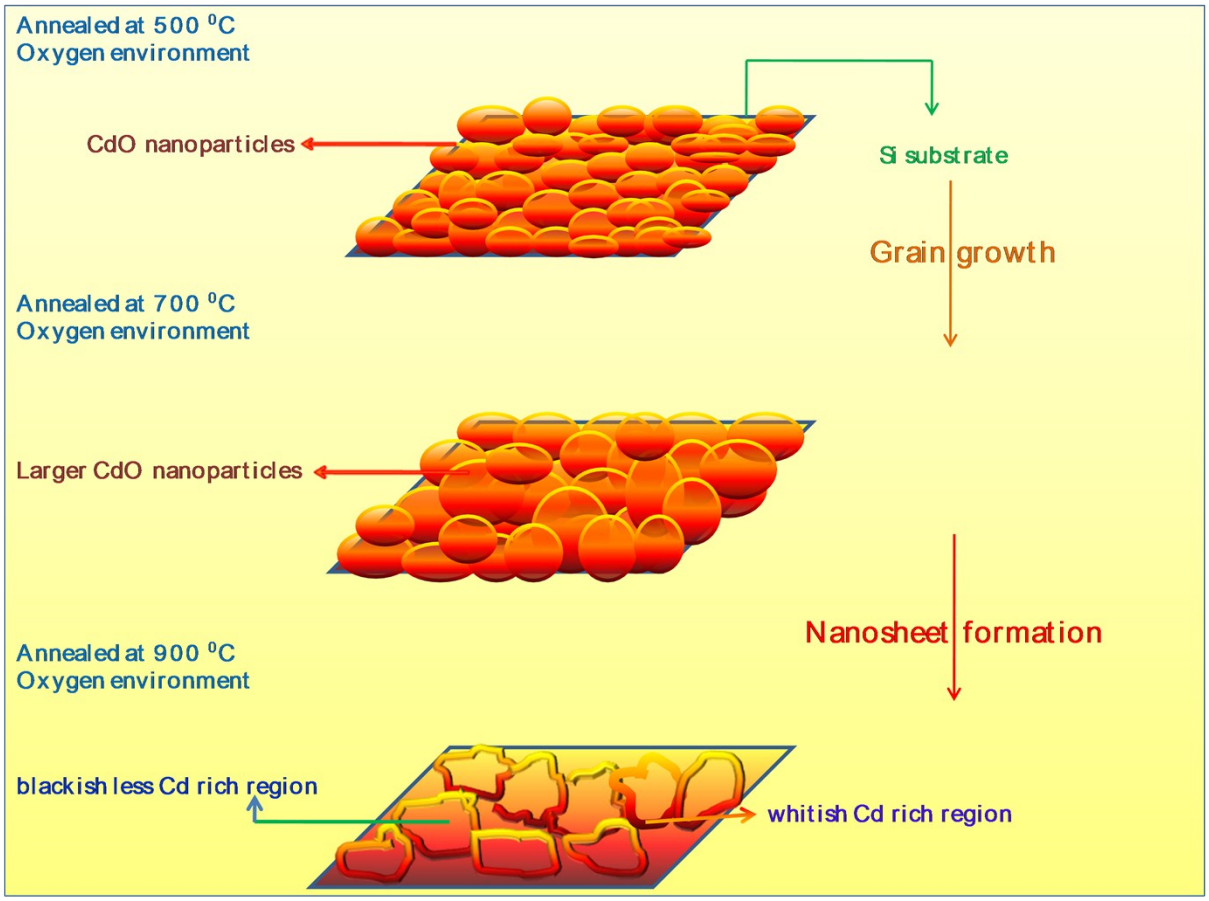

Figure 4S: Schematic illustration of nanosheet formation