Electronic Supplementary Material (ESI) for Nanoscale.


# Orbital hybridization induced band offset phenomena in $Ni_xCd_{1-x}O$ thin films

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**Table (S1):** Calculated and obtained numerical values of different parameters

| Sample name | 2θ Position of (111) peak (degree) | FWHM of (111) peak | 2θ Position of (220) peak (degree) | Effective reduced mass (atomic weight) | Compositional percentage from RBS measurements | | |
|---|---|---|---|---|---|---|---|
| | | | | | Cd% | O% | Ni% |
| 4Cd | 33.06 | 0.42 | 55.42 | 14.00 | 49.8 | 49.2 | 0 |
| 3% Ni | 33.04 | 0.60 | 55.43 | 13.98 | 49 | 49 | 1.9 |
| 5% Ni | 33.10 | 0.63 | 55.44 | 13.96 | 46.6 | 49.9 | 3.4 |
| 10% Ni | 33.13 | 0.88 | 55.51 | 13.92 | 44.3 | 50 | 5.9 |
| 20% Ni | 33.24 | 0.87 | 55.66 | 13.82 | 36.5 | 52.9 | 10.6 |
| 40% Ni | 33.34 | 1.39 | 56.04 | 13.60 | 24.1 | 51.9 | 24.1 |
| 80% Ni | *n.a.* | *n.a.* | *n.a.* | 13.00 | 5.1 | 57.7 | 37.2 |
| 100% Ni | *n.a.* | *n.a.* | *n.a.* | 12.57 | 0 | 58.1 | 41.9 |

**n.a.** = Not Applicable

**Table (S2):** Carrier concentration value with increasing Ni doping percentage for $Ni_xCd_{1-x}O$ thin films

| Sample name | Carrier concentration (/cc) |
|---|---|
| 4Cd | -8.400E+19 |
| 3% Ni | -6.587E+19 |
| 5% Ni | -5.487E+19 |
| 10% Ni | -2.196E+19 |
| 20% Ni | -1.887E+19 |
| 40% Ni | N.A. |

Reference: Arkaprava Das *et al.*, Electronic excitation induced anomalous band gap enhancement in $Ni_xCd_{1-x}O$ thin films; Vacuum 146 (2017) 287-296

**Table (S3):** Fitting parameters for O 1s, Ni 2p and Cd 3d XPS spectra

| sample | Peak position (eV) | area | fwhm |
|---|---|---|---|
| 4Cd (Cd 3d) | | | |
| CdO | 403.5 | 58900 | 1.46 |
| $CdO_2$ | 404.4 | 22589 | 1.11 |
| 4Cd (O 1s) | | | |
| $Cd(OH)_2$/ $CdCO_3$ | 530.5 | 10978 | 1.64 |
| CdO | 527.9 | 4704 | 0.91 |
| $CdO_2$ | 528.8 | 2709 | 1.29 |
| 5% Ni (Cd 3d) | | | |
| CdO | 403.5 | 58307 | 1.45 |
| $CdO_2$ | 404.4 | 22352 | 1.09 |
| 5% Ni (O 1s) | | | |
| $Cd(OH)_2$/ $CdCO_3$ | 530.5 | 10838 | 1.64 |
| CdO | 527.9 | 4600 | 0.91 |
| $CdO_2$ | 528.8 | 2689 | 1.29 |
| 5% Ni (Ni 2p) | | | |
| $Ni^0$ | 851.5 | 197 | 0.8 |
| $Ni^{2+}$ | 853.6 | 1259 | 3.1 |
| Satellite | 859.9 | 1143 | 5.8 |
| Satellite | 871.9 | 2198 | 13.9 |
| | | | |
| 10% Ni (Cd 3d) | | | |
| CdO | 403.4 | 53205 | 1.15 |
| $CdO_2$ | 404.3 | 31243 | 1.37 |
| 10% Ni (O 1s) | | | |
| $Cd(OH)_2$/ $CdCO_3$ | 530.6 | 7728 | 1.74 |
| CdO | 528.1 | 8263 | 0.93 |
| $CdO_2$ | 528.9 | 1982 | 0.94 |
| 10% Ni (Ni 2p) | | | |
| $Ni^0$ | 851.6 | 2771 | 1.09 |
| $Ni^{2+}$ | 853.6 | 5492 | 2.9 |
| Satellite | 859.7 | 7844 | 7.3 |
| Satellite | 871.1 | 5605 | 6.1 |
| Satellite | 878.5 | 3302 | 6.2 |
| 40% Ni (Cd 3d) | | | |
| CdO | 403.6 | 15848 | 1.24 |
| $CdO_2$ | 404.5 | 10064 | 1.23 |
| 40% Ni (O 1s) | | | |

| | | | |
|---|---|---|---|
| $Cd(OH)_2$/ $CdCO_3$ | 530.5 | 7646 | 1.86 |
| CdO | 528.4 | 4173 | 1.09 |
| $CdO_2$ | 528.8 | 1958 | 0.84 |
| 40% Ni (Ni 2p) | | | |
| $Ni^0$ | 851.8 | 9828 | 0.9 |
| $Ni^{2+}$ | 852.8 | 19043 | 2.9 |
| $Ni^{3+}$ | 855.3 | 5381 | 2.4 |
| Satellite | 859.4 | 19027 | 6.6 |
| Satellite | 872.0 | 19131 | 9 |
| Satellite | 879.6 | 4444 | 5 |
| | | | |
| 100% Ni (O 1s) | | | |
| NiO | 529.7 | 12248 | 1.14 |
| $Ni(OH)_2$ | 531.3 | 7300 | 1.92 |
| 100% Ni (Ni 2p) | | | |
| $Ni^0$ | 852.5 | 12716 | 0.9 |
| $Ni^{2+}$ | 854 | 33000 | 2.8 |
| $Ni^{3+}$ | 856.4 | 13694 | 2.6 |
| Satellite | 860.5 | 37560 | 6.8 |
| Satellite | 873.3 | 33647 | 9.4 |
| Satellite | 880.8 | 8343 | 4.6 |