SUPPLEMENTARY MATERIAL TO THE PAPER

**MgCo2-D2 and MgCoNi-D2 systems synthesized at high pressures**

**and interaction mechanism during the HDDR processing**

by

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**Crystal structure data for compounds participating in the phase-structural transformations**

**Table S1**

Crystal structure data for Co

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| T = 27 °C | Atoms | Sites | *x/a* | *y/b* | *z/c* | occ. |
| LT hcp CoSpace group | Co | 2c | 1/3 | 2/3 | 1/4 | 1 |
| *P63/mmc* (No. 194) |  |  |  |  |  |  |
| *a* =0.2507 nm*c* =0.4076 nm |  |  |  |  |  |  |
|  |  |  |  |  |  |  |
| T = 500 °C |  |  |  |  |  |  |
| HT fcc CoSpace group | Co | 4a | 0 | 0 | 0 | 1 |
| *Fm*$\overbar{3}$*m* (No. 225) |  |  |  |  |  |  |
| *a*=0.3560 nm |  |  |  |  |  |  |

**Table S2**

Crystal structure data for Mg2CoD5

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| T = 27 °C | Atoms | Sites | *x/a* | *y/b* | *z/c* | occ. |
| LT -Mg2CoD5Space group | Mg1Mg2 | 2a2b | ¾¾  | ¼¼  | ½0 | 11 |
| *P4/nmm* (No. 129) | Co | 2c | ¼  | ¼  | 0.2470 | 1 |
| *a* =0.4468 nm | D1 | 2c | ¼  | ¼  | 0.0028 | 1 |
| *c* =0.6577 nm | D2 | 8j | 0.0121 | 0.0121 | 0.2743 | 1 |
|  |  |  |  |  |  |  |
| HT -Mg2CoD5T = 250 °C | MgCo | 8c4a | ¼ 0 | ¼ 0 | ¼ 0 | 11 |
| Space group | D | 24e | 0.2368 | 0 | 0 | 0.83 |
| *Fm*$\overbar{3}$*m* (No. 225) |  |  |  |  |  |  |
| *a* =0.646 nm |  |  |  |  |  |  |
|  |  |  |  |  |  |  |

**Table S3**

Crystal structure data for MgCo2

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| T = 500 °C | Atoms | Sites | *x/a* | *y/b* | *z/c* | occ. |
| Space group | Mg | 4f | 1/3  | 2/3 | 0.5629 | 1 |
| *P63/mmc* (No. 194) | Co1 | 2a | 0.1697 | 0.3394 | 1/4 | 1 |
| *a* =0.4895 nm | Co2 | 6h | 0 | 0 | 0 | 1 |
| *c* =0.7998 nm |  |  |  |  |  |  |
|  |  |  |  |  |  |  |

**Table S4**

Crystal structure data for MgCo

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| T = 500 °C | Atoms | Sites | *x/a* | *y/b* | *z/c* | occ. |
| Space group | Mg | 48f | 0.4209 | 1/8 | 1/8 | 1 |
| *Fd*$\overbar{3}$*m* (No. 227) | Co1 | 16c | 0 | 0 | 0 | 1 |
| *a* =1.1555 nm | Co2 | 32e | 0.2020 | 0.2020 | 0.2020 | 1 |
|  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |

**Table S5**

Crystal structure data for Mg

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| T = 300 °C | Atoms | Sites | *x/a* | *y/b* | *z/c* | occ. |
| Space group | Mg | 2c | 1/3 | 2/3 | 1/4 | 1 |
| *P63/mmc* (No. 194) |  |  |  |  |  |  |
| *a* =0.3233 nm |  |  |  |  |  |  |
| *c* =0.5252 nm |  |  |  |  |  |  |

**Table S6**

Crystal structure data for MgO

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| T = 27°C | Atoms | Sites | *x/a* | *y/b* | *z/c* | occ. |
| Space group | Mg | 4a | 0 | 0 | 0 | 1 |
| *Fm*$\overbar{3}$*m* (No. 225) | O | 4b | 1/2 | 1/2 | 1/2 | 1 |
| *a* =0.4212 nm |  |  |  |  |  |  |
|  |  |  |  |  |  |  |

Rietveld refinements data for the MgCo2D2.5 systemat 27°C - 500°C



Rwp=7.0%, Rp=4.8%, χ2=9.1

Fig. S1. NPD pattern of the MgCo2D2.5 system at 27°C.



Rwp=7.5%, Rp=5.0%, χ2=8.6

Fig. S2. NPD pattern of the MgCo2D2.5 system at 150°C.



Rwp=6.9%, Rp=4.7%, χ2=7.6

Fig. S3. NPD pattern of the MgCo2D2.5 system at 200°C.



Rwp=6.7%, Rp=4.6%, χ2=6.8

Fig. S4. NPD pattern of the MgCo2D2.5 system at 250°C.



Rwp=8.0%, Rp=5.6%, χ2=12.2

Fig. S5. NPD pattern of the MgCo2D2.5 system at 300°C.



Rwp=8.0%, Rp=5.5%, χ2=10.2

Fig. S6. NPD pattern of the MgCo2D2.5 system at 350°C in vacuum.



Rwp=8.1%, Rp=5.5%, χ2=10.3

Fig. S7. NPD pattern of the MgCo2D2.5 system at 400°C in vacuum.



Rwp=7.4%, Rp=5.1%, χ2=8.8

Fig. S8. NPD pattern of the MgCo2D2.5 system at 450°C in vacuum.



Rwp=5.9%, Rp=4.3%, χ2=5.5

Fig. S9. NPD pattern of the MgCo2D2.5 system at 500°C in vacuum.