

Article

Study on Microstructure and Hydrogen Storage Properties of $\text{Mg}_{80}\text{Ni}_{16-x}\text{Al}_x\text{Y}_4$ ($x = 2, 4, 8$) Alloys

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Table S1. Crystal structures of intermetallic compounds in the present study.

| Phase | Space group | Latter Parameter | | | | | | ICSD |
|-------------------------------------|----------------------|------------------|--------|--------|--------------------|-------------------|--------------------|--------|
| | | a(Å) | b(Å) | c(Å) | $\alpha(^{\circ})$ | $\beta(^{\circ})$ | $\gamma(^{\circ})$ | |
| Mg | P6 ₃ /mmc | 3.2061 | 3.2061 | 5.2091 | 90 | 90 | 120 | 77908 |
| Mg ₂ Ni | P6 ₂ 22 | 5.205 | 5.205 | 13.236 | 90 | 90 | 120 | 30714 |
| YMgNi ₄ | F-43m | 7.01 | 7.01 | 7.01 | 90 | 90 | 90 | 107033 |
| AlNi | Pm-3m | 2.882 | 2.882 | 2.882 | 90 | 90 | 90 | 58037 |
| Al ₃ Ni ₂ Y | P6/mmm | 9.006 | 9.006 | 4.070 | 90 | 90 | 120 | 54425 |
| Mg ₂ NiH _{0.29} | P6 ₂ 22 | 5.256 | 5.256 | 13.435 | 90 | 90 | 120 | 49534 |
| Mg ₂ NiH ₄ | Fm-3m | 6.508 | 6.508 | 6.508 | 90 | 90 | 90 | 38409 |
| MgH ₂ | P4 ₂ /mnm | 4.514 | 4.514 | 2.992 | 90 | 90 | 90 | 161962 |
| YH ₂ | Fm-3m | 5.2032 | 5.2032 | 5.2032 | 90 | 90 | 90 | 44097 |
| YH ₃ | P6 ₃ /mmc | 3.672 | 3.672 | 6.646 | 90 | 90 | 120 | 41548 |

Table S2. Unit cell parameters of the original alloy.

| Phase | | a(Å) | c(Å) |
|-----------------|-----------------------------------|--------|---------|
| Al ₂ | Mg | 3.2128 | 5.2129 |
| | Mg ₂ Ni | 5.2467 | 13.3660 |
| | AlNi | 2.9064 | |
| | YMgNi ₄ | 7.1266 | |
| Al ₄ | Mg | 3.2133 | 5.2122 |
| | Mg ₂ Ni | 5.2341 | 13.3653 |
| | AlNi | 2.8988 | |
| | YMgNi ₄ | 7.0941 | |
| Al ₈ | Mg | 3.2108 | 5.2098 |
| | Mg ₂ Ni | 5.2200 | 13.3800 |
| | Al ₃ Ni ₂ Y | 9.0064 | 4.0675 |

(Since LPSO does not have a standard structure file, it is not possible to accurately determine the unit cell parameters.)

Table S3. Kinetic data points.

| Samples | Temperature (K) | lnk |
|------------------------------------------------------------------|-----------------|----------|
| Mg ₈₀ Ni ₁₄ Al ₂ Y ₄ | 473.15 | -4.7489 |
| | 523.15 | -3.21363 |
| | 573.15 | -2.71963 |
| Mg ₈₀ Ni ₁₂ Al ₄ Y ₄ | 473.15 | -5.92776 |
| | 523.15 | -4.19368 |
| | 573.15 | -3.82636 |
| Mg ₈₀ Ni ₈ Al ₈ Y ₄ | 473.15 | -5.74091 |
| | 523.15 | -3.96902 |
| | 573.15 | -3.10864 |

Table S4. Thermodynamic data points.

| Samples | Temperature (K) | P _H (bar) |
|------------------------------------------------------------------|-----------------|----------------------|
| Mg ₈₀ Ni ₁₄ Al ₂ Y ₄ | 473.15 | 0.07 |
| | 523.15 | 0.49 |
| | 573.15 | 2.16 |
| Mg ₈₀ Ni ₁₂ Al ₄ Y ₄ | 473.15 | 0.06 |
| | 523.15 | 0.42 |
| | 573.15 | 1.92 |
| Mg ₈₀ Ni ₈ Al ₈ Y ₄ | 473.15 | 0.06 |
| | 523.15 | 0.20 |
| | 573.15 | 1.90 |