Supplemental

Electron Backscatter Diffraction Studies on the Formation of Superlattice Metal Hydride Alloys

Shuli Yan, Kwo-Hsiung Young, Xin Zhao, Zhi Mei and K. Y. Simon Ng

1. Influence of Misorientation on the Quality of EBSD Pattern

A SEM image of the 32-h annealed sample is shown in Figure S1a. EBSD mapping was performed in the area enclosed by the green rectangle in Figure S1a. Figure S1b shows the distribution of the $NbCr_2$ grains, and Figure S1c provides the color assignment. Only three large grains are discovered in the area enclosed by the green rectangle. We collected the EBSD diffraction data in spots A, B, and C in the green grain.

EBSD pattern of spot A has the most diffraction lines among those of all three spots. Intensities of the diffraction lines are different. Generally speaking, band intensity could be influenced by camera resolution, background subtraction, sample surface, and some other parameters, leading to the difference in numbers of diffraction lines distinguished by naked eye and computer.

Spots B and C represent the crystals with misorientation less than 2° compared to spot A (A2, B2, and C2 in Figure S2). B1 and C1 of Figure S2 show that intensities of the diffraction lines are different compared to those in A1 of Figure S2. Moreover, other variations are observed: some lines disappear; new lines appear; some lines move parallelly; some lines rotate slightly; and widths of some lines change. Therefore, patterns may appear to be different by naked eye, especially C1 of Figure S2.

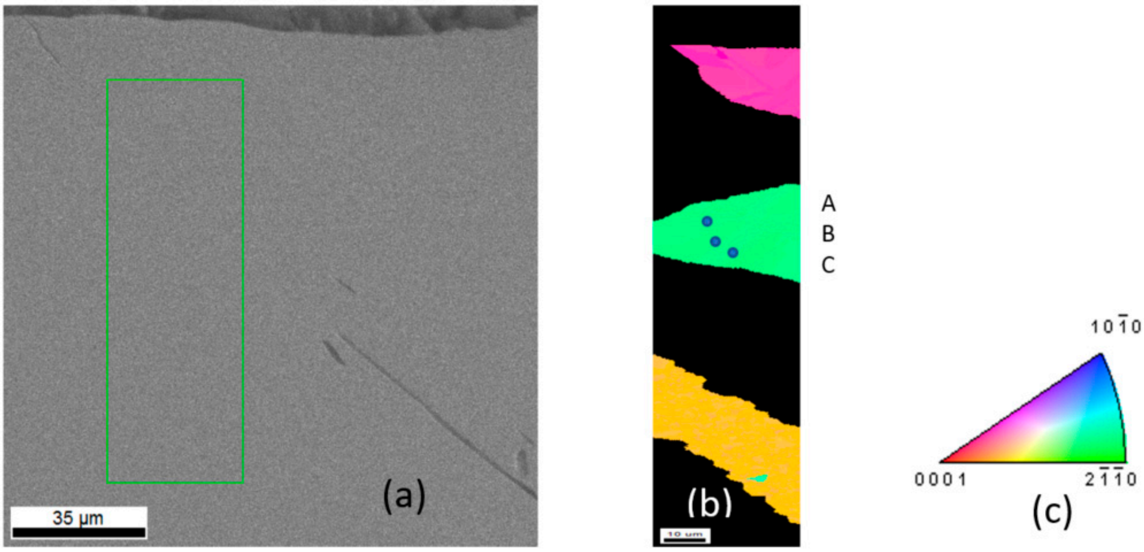


Figure S1. (**a**) SEM image of the 32-h annealed sample, (**b**) EBSD mapping of $NbCr_2$, and (**c**) color assignment.

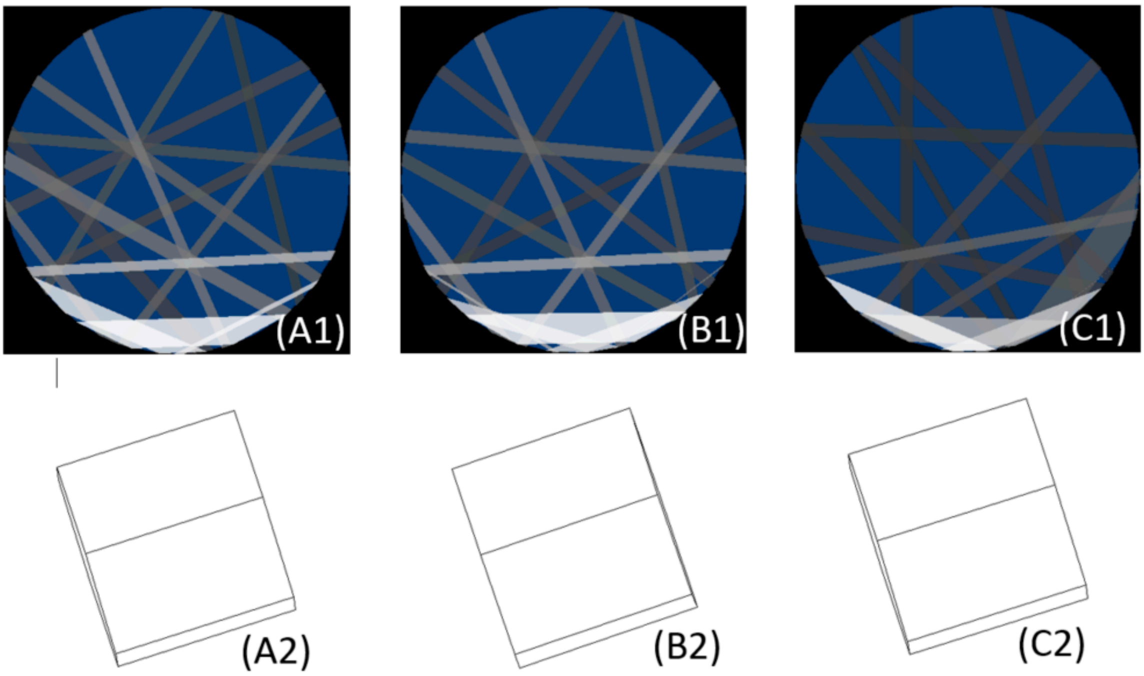
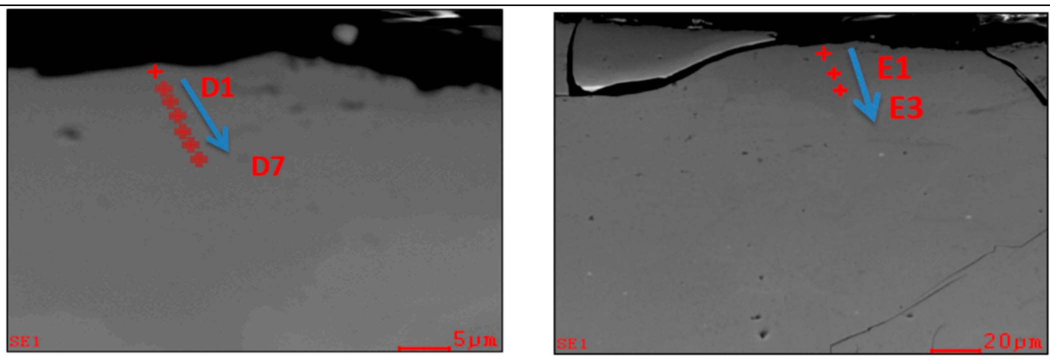


Figure S2. EBSD diffraction patterns (A1, B1, C1) and corresponding crystals (A2, B2, C2) for spots A, B, and C in Figure S1b.

2. Existence of the Mg Phase

Formation of an isolated Mg phase within the alloy bulk by the inter-diffusion of Mg is unlikely. However, EBSD patterns of some spots with perfect fitting to that of the crystalline Mg in several treated alloys are observed, and EDS reveals very high Mg-content in those spots. For example, in two areas of the 4-h annealed sample, EDS measurements were performed (Figure S3). The EDS results are summarized in Table S1 and show high Mg-content in some spots. Since the solubilities of La and Ni in Mg are negligible, these areas with high Mg-content (> 75 at%) are considered to be the pure Mg phase with the La and Ni signals from the neighboring phases.



(**a**) (**b**)

Figure S3. SEM images from two areas of the 4-h annealed sample.

Table S1. Chemical compositions (in at%) from spots D1 to D7 and E1 to E3 of the 4-h annealed sample (Figure S3).

Spot	Mg	La	Ni	Ni/(La + Mg)
D1	58.46	8.25	33.29	0.50
D2	86.30	6.04	7.65	0.08
D3	82.10	5.55	12.34	0.14
D4	80.79	5.72	13.49	0.16
D5	75.57	7.31	17.13	0.21
D6	12.88	11.8	75.32	3.05
D7	10.65	12.03	77.32	3.41
E1	81.32	7.78	10.90	0.12
E2	76.02	12.22	11.76	0.13
E3	10.99	12.23	76.78	3.31