Supplemental Information

Superhard Tungsten Diboride-Based Solid Solutions

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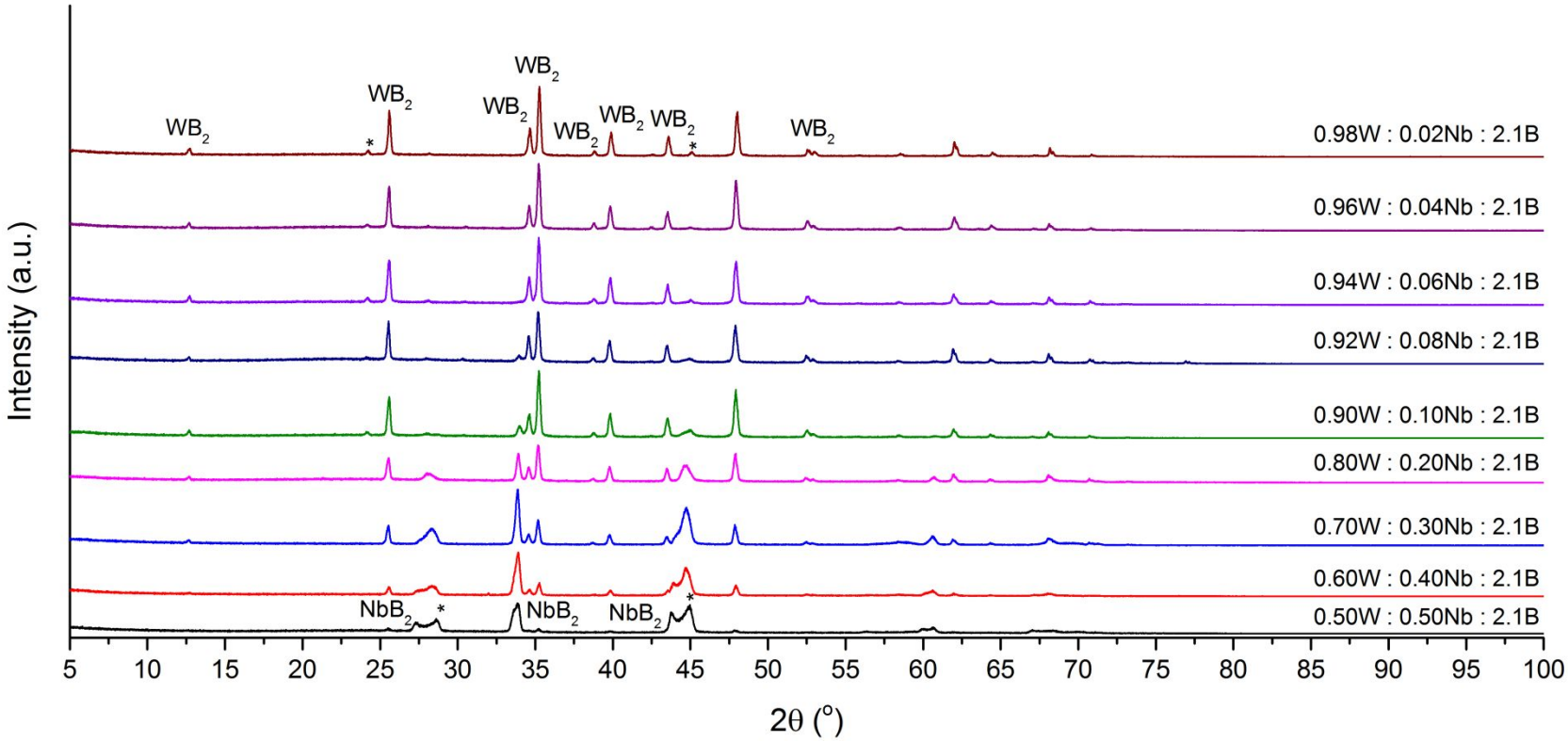
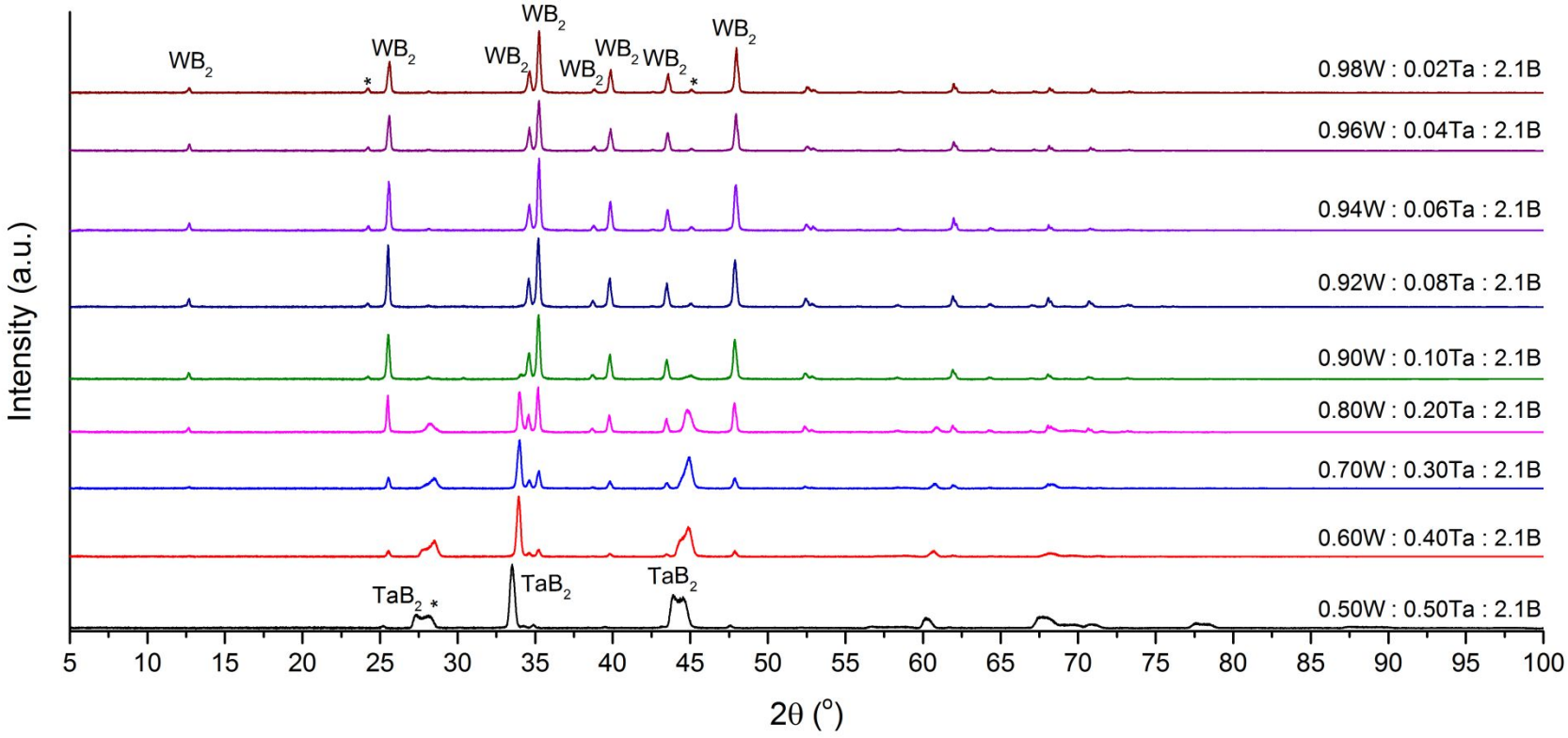

Intensity (a.u.)
WB2
NbB2
*
0.98W : 0.02Nb : 2.1B
0.96W : 0.04Nb : 2.1B
0.94W : 0.06Nb : 2.1B
0.92W : 0.08Nb : 2.1B
0.90W : 0.10Nb : 2.1B
0.80W : 0.20Nb : 2.1B
0.70W : 0.30Nb : 2.1B
0.60W : 0.40Nb : 2.1B
0.50W : 0.50Nb : 2.1B
5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100
2θ (°)

(a)



(b)

Figure S1. Powder XRD patterns of: (a) $W_{1-x}Nb_xB_2$ and (b) $W_{1-x}Ta_xB_2$, where x = 0.02, 0.04, 0.06, 0.08, 0.10, 0.20, 0.30, 0.40 and 0.50. For (a), the solubility limit of Nb in WB_2 is < 8 at. % Nb. At increasing concentration of Nb, the WB_2 phase decreases and niobium diboride (NbB_2) increases. 50 at. % Nb contains a combination of WB_4 and NbB_2. For (b), the solubility limit of Ta in WB_2 is < 10 at. % Ta. Above the solubility limit, the WB_2 phase decreases and tantalum diboride (TaB_2) increases. 50 at. % Ta contains both WB_4 and TaB_2. The asterisk (*) denotes visible WB_4 peaks at low concentrations of Nb and Ta substitution.

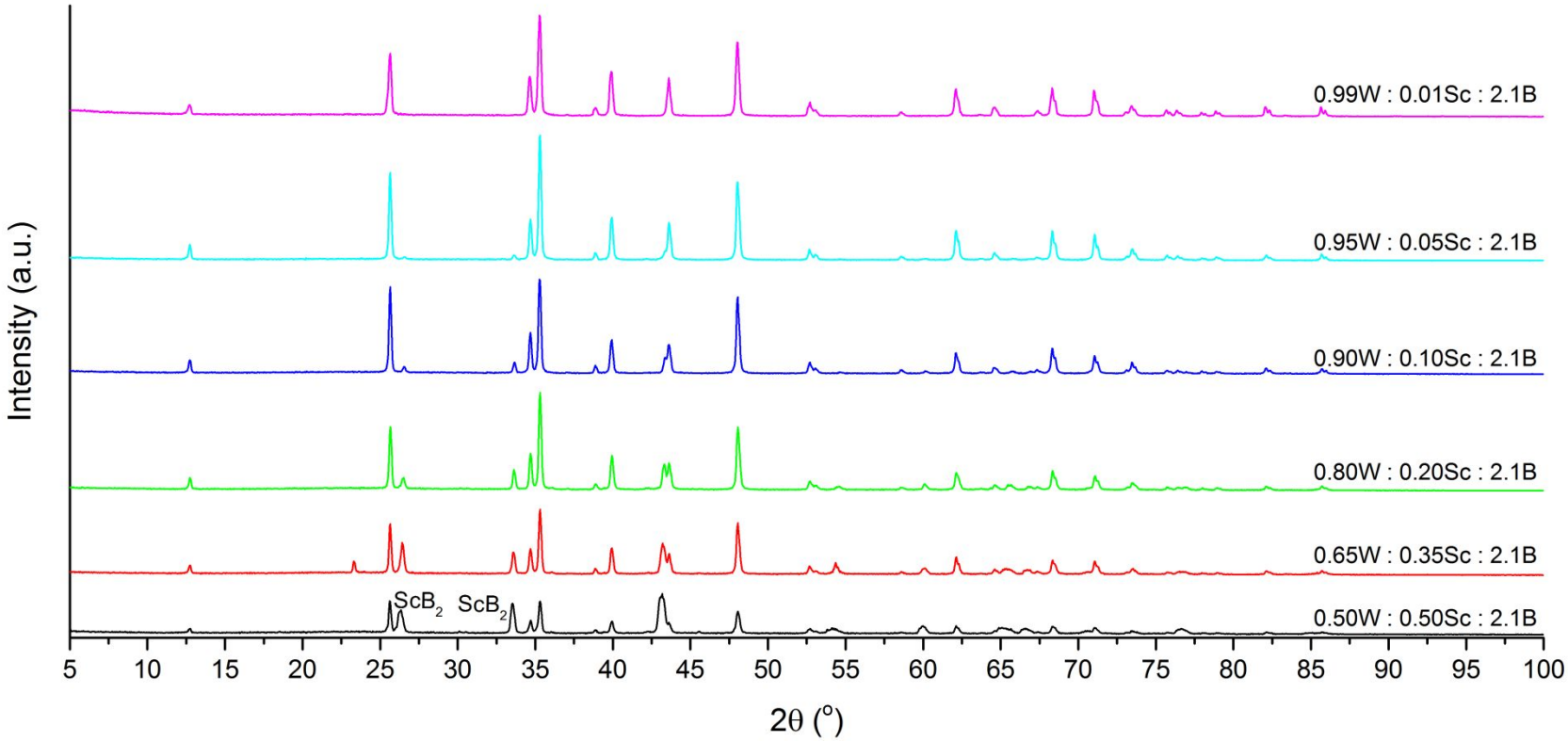


Figure S2. Powder XRD patterns of: $W_{1-x}Sc_xB_2$, where x = 0.01, 0.05, 0.10, 0.20, 0.35, and 0.50. Above 1 at. % Sc, a secondary phase, ScB_2 (JCPDS 03-065-6646) increases with increasing scandium substitution.

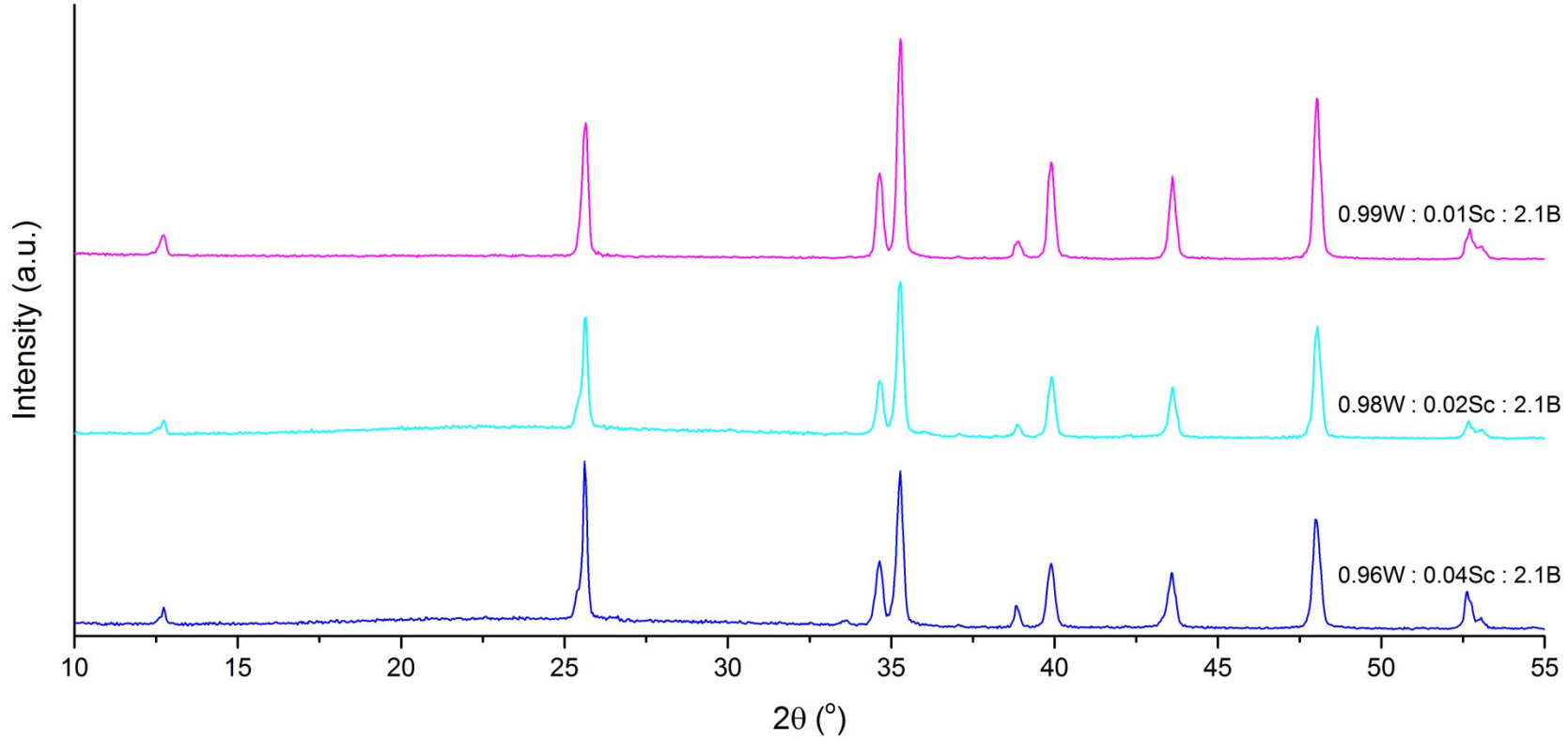


Figure S3. Powder XRD patterns of: $W_{1-x}Sc_xB_2$, where x = 0.01, 0.02 and 0.04 (top to bottom) and M : B = 1 : 2.1. The solubility limit of Sc in WB_2 is < 4 at. % Sc. A minimum amount of 1 at. % Sc was used to stabilize phase-pure WB_2 by PXRD analysis.

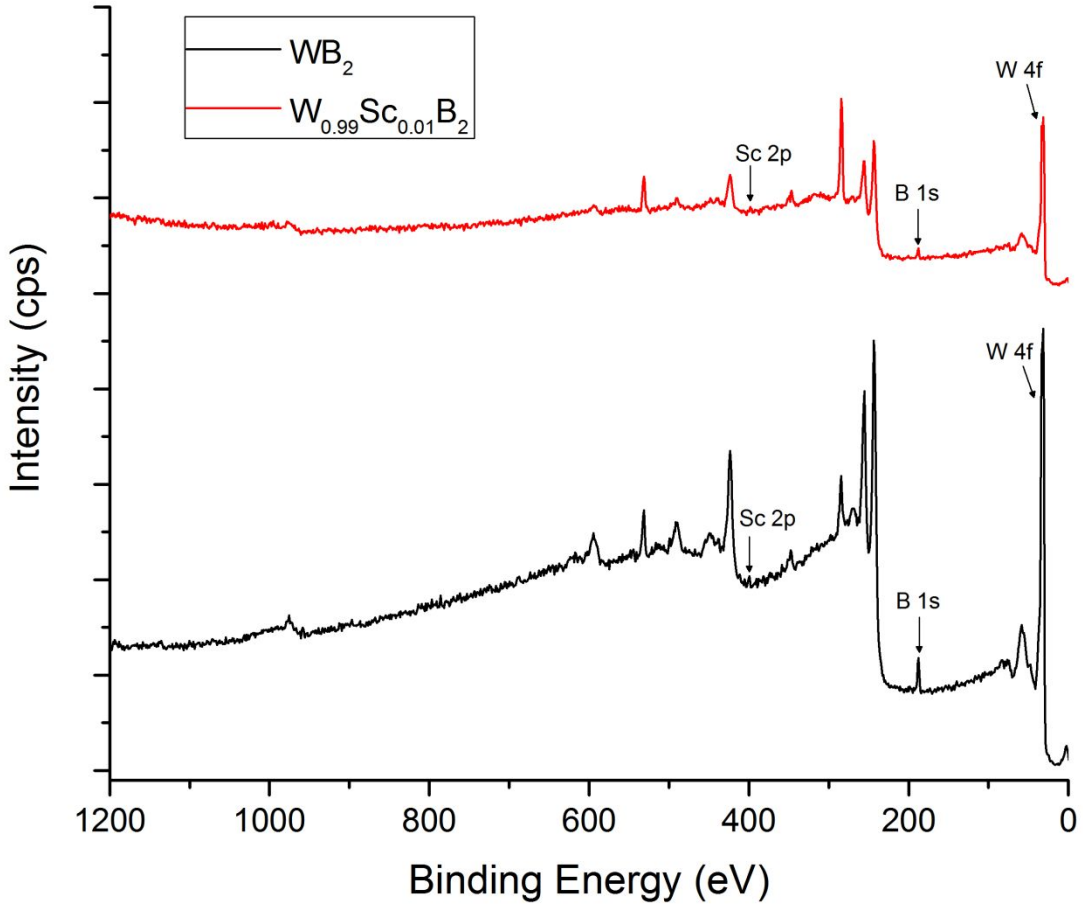
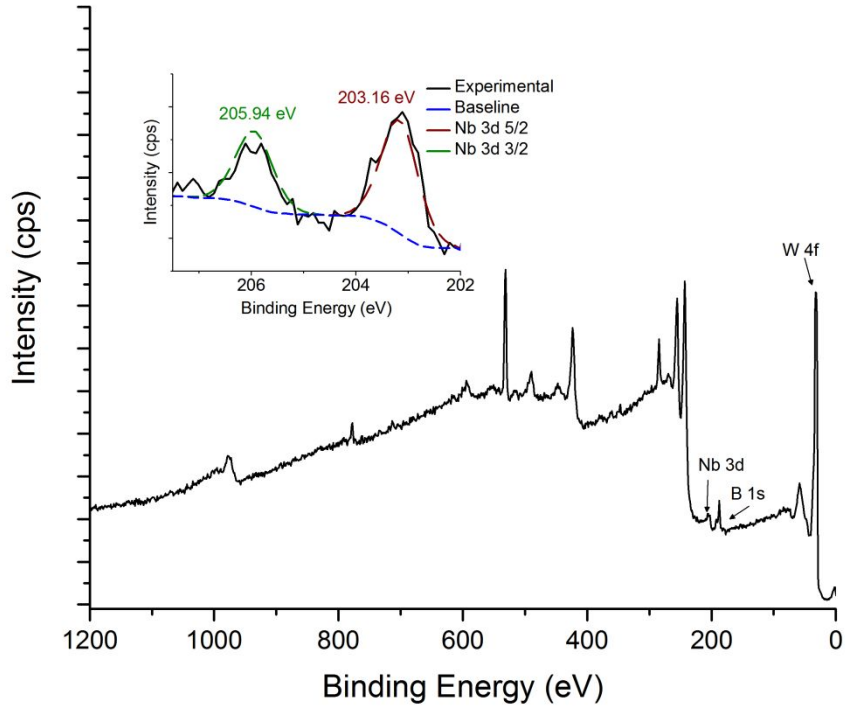
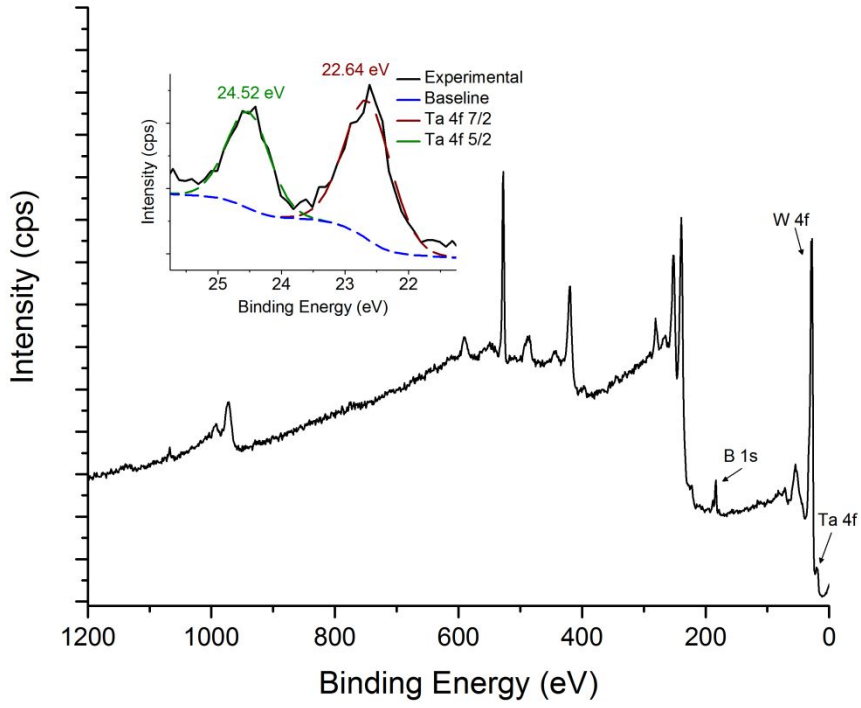


Figure S4. Survey XPS spectrum of WB_2 and $W_{0.99}Sc_{0.01}B_2$ polished samples having nominal compositions of M : B = 1 : 2.1. W 4f, Sc 2p, and B 1s electron regions are labeled.



(a)



(b)

Figure S5. Survey XPS spectrum of (a) $W_{0.94}Nb_{0.06}B_2$ and (b) $W_{0.92}Ta_{0.08}B_2$ polished samples having nominal compositions of M : B = 1 : 2.1. Electron regions of interest are labeled. Binding energy regions for the Nb 3d peaks and Ta 4f peaks are included as inset graphs in (a) and (b), respectively.

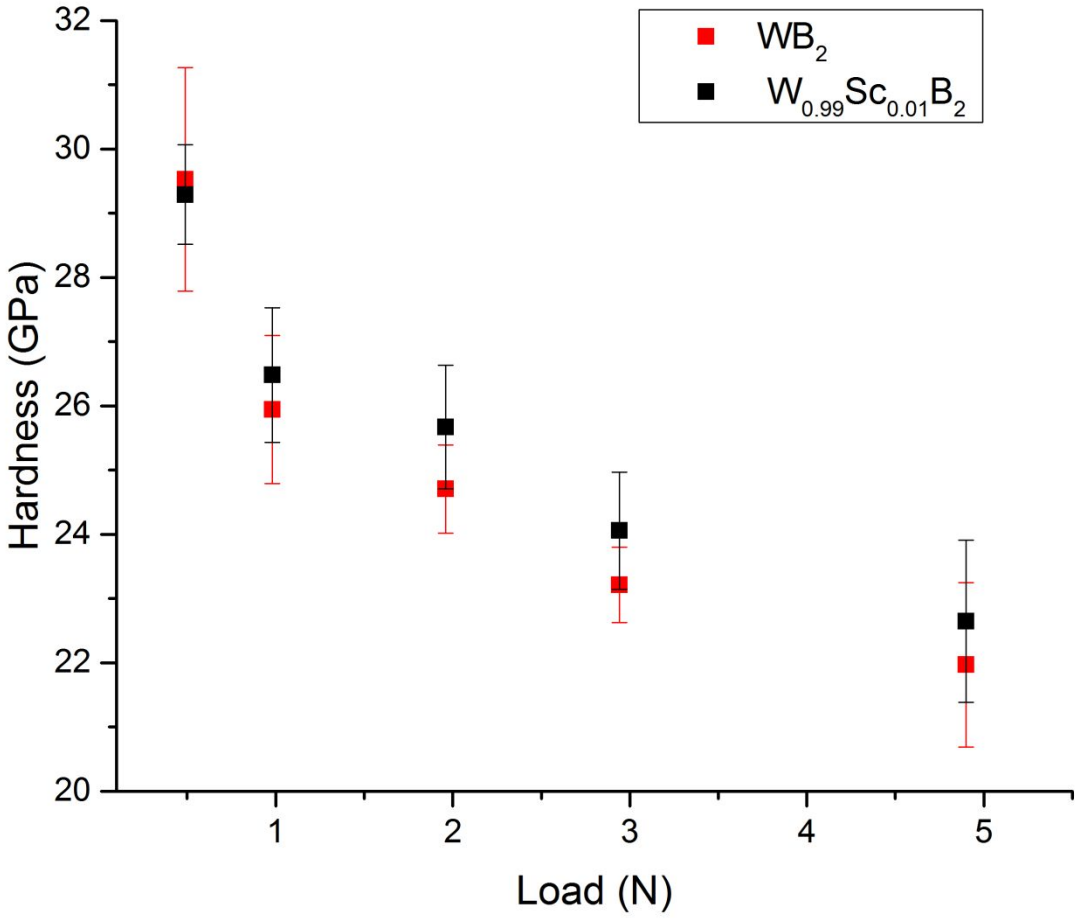


Figure S6. Vickers hardness measurements at applied loads ranging from 0.49 N to 4.9 N for 0 at. % and 1 at. % Sc in WB_2. Hardness values for both samples are within error at each load, indicating that the presence of WB_4 has minimal effect on overall hardness.

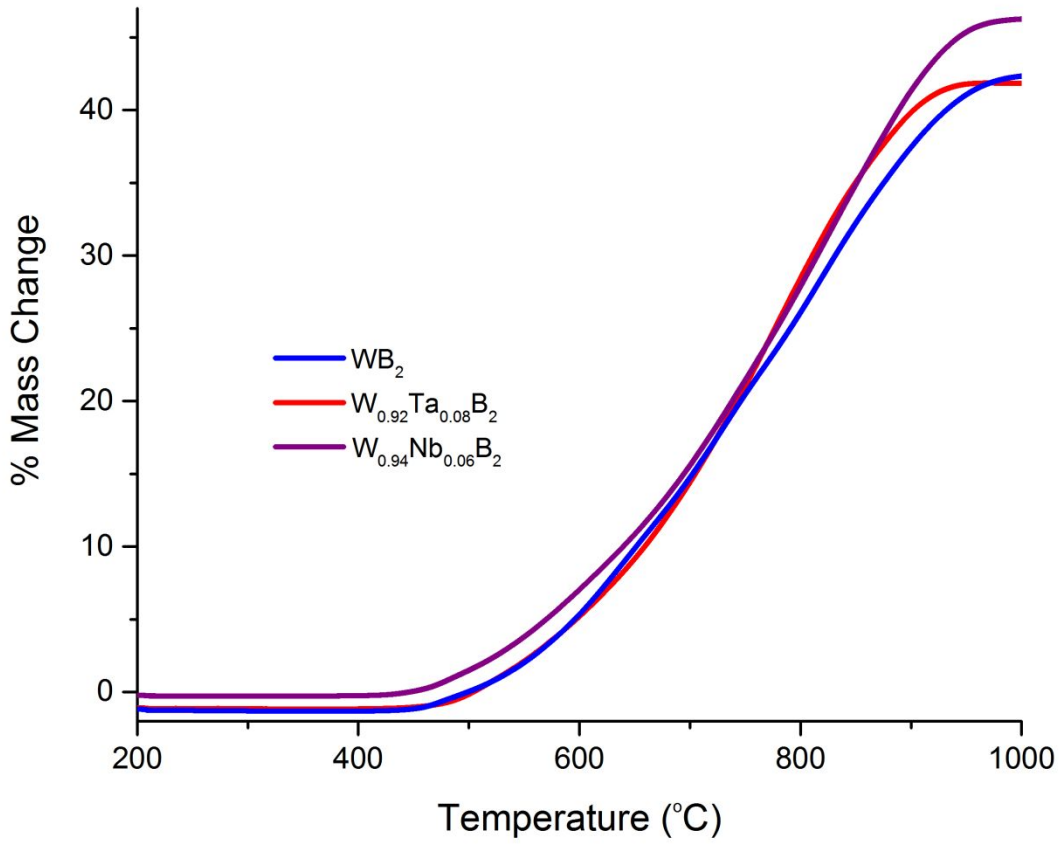


Figure S7. Thermal gravimetric analysis data for WB_2 and the hardest WB_2 solid solutions with Ta and Nb. These data indicate that the samples are thermally stable in air up to a temperature of ~520 °C, ~570 °C and ~550 °C for WB_2, $W_{0.92}Ta_{0.08}B_2$, and $W_{0.94}Nb_{0.06}B_2$, respectively.