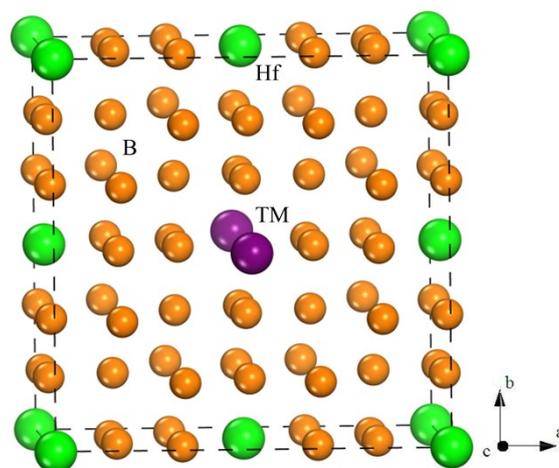


## Supplementary Materials



Structural configuration of  $\text{HfB}_{12}$  with alloying elements. The green, brown and purple spheres represent the Hf, B and TM atoms, respectively.

Atomic position:

Hf:  $4a(0, 0, 0)$

B:  $48i(0.50, 0.1699, 0.1699)$

Reference:

- <sup>1</sup> H. Werheit, V. Filipov, K. Shirai, H. Dekura, N. Shitsevalova, U. Schwarz, M. Armbruster, *J. Phys.: Condens. Matter* **2011**, 23, 065403.
- <sup>2</sup> N. Korozlu, K. Colakoglu, E. Deligoz, S. Aydin, *J. Alloys. Compd.* **2013**, 546, 157-164.