First Principles investigation of Transition Metal Solubility in Titanium-Boride

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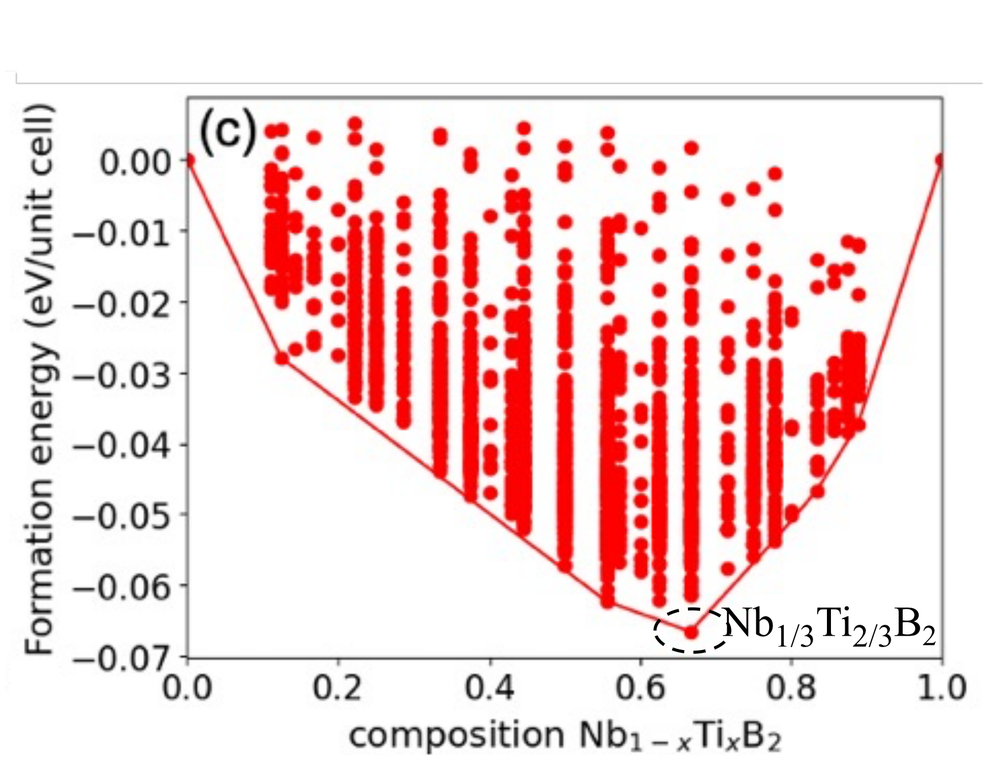
Motivation

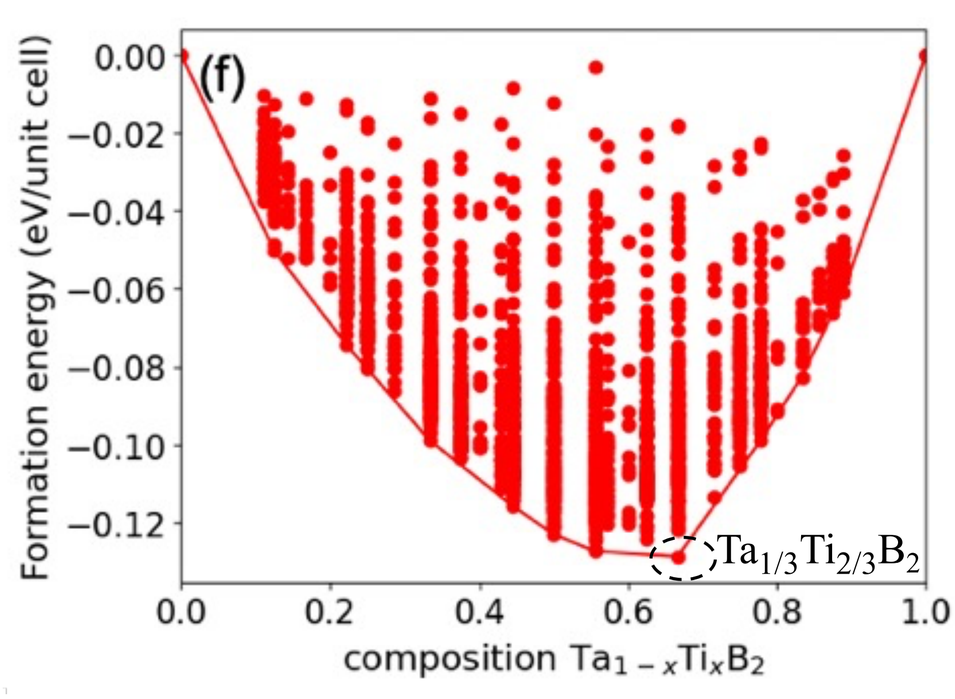
- TiB_2 is a promising nucleation catalyst for the hydration of MgB_2 [1]
- MgB_2 and TiB_2 share the same crystal structure, but with slightly different lattice constants [2]
- Tailoring the lattice constant of TiB_2 to match MgB_2 is attractive to
  - provide ideal nucleation sites for MgB_2 and, thus,
  - reduce the activation energy for dehydrogentation of Magnesium Borohydride

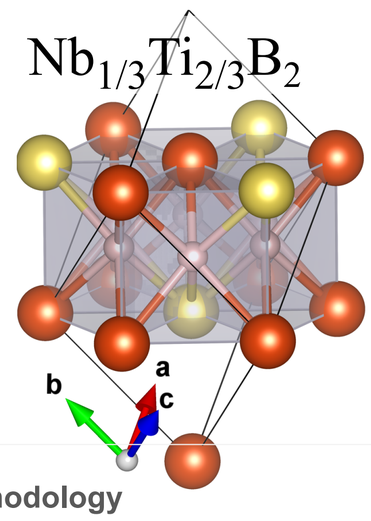
Table 1. Crystal structure of diborides [2].

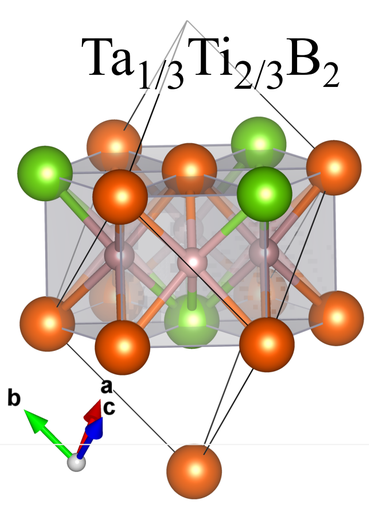
Diborides	Lattice parameters (Å)	Formation energy (eV/atom)	Space group
TiB_2	a=b=3.035 c= 3.223	-1.056	P6/mmm [191]
MgB_2	a=b=3.074 c=3.534	-0.130	
ScB_2	a=b=3.146 c=3.524	-0.839	
YB_2	a=b=3.301 c=3.854	-0.629	
ZrB_2	a=b=3.180 c=3.545	-0.987	
HfB_2	a=b=3.149 c=3.480	-1.805	
NbB_2	a=b=3.112 c=3.337	-0.694	
TaB_2	a=b=3.097 c=3.343	-0.663	

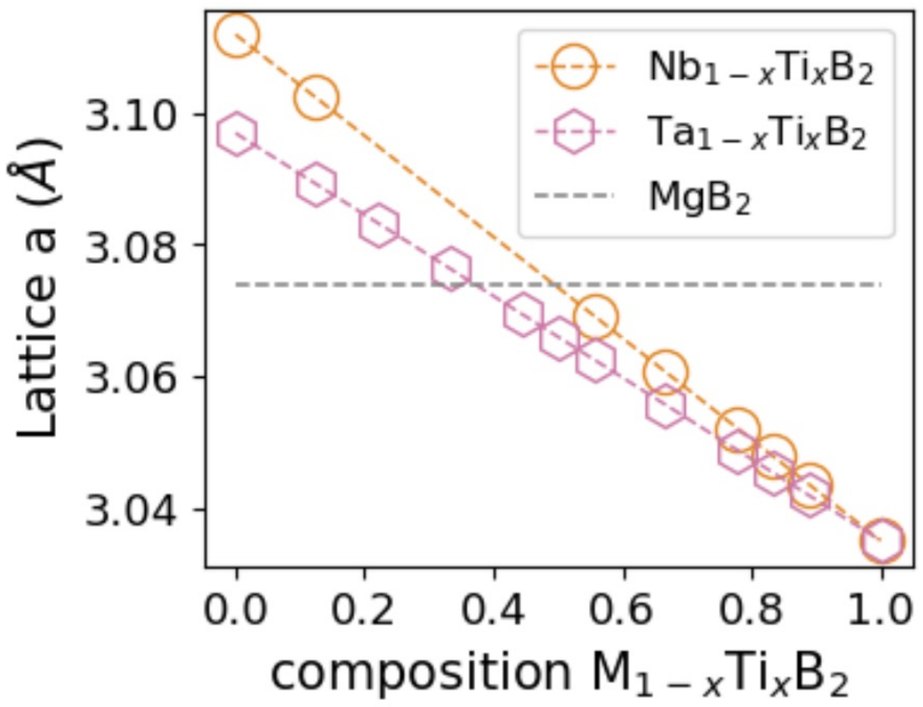
Hexagonal Prism











Methodology

- Total Energy calcualtions with VASP within the GGA-PWE approximation to DFT
- Cluster expansion of the configurational degrees of freedom with CASM [3]

Conclusion

- (Nb-Ti)B_2 and (Ta-Ti)B_2 are predicted to form solid solutions
- Lattice constants vary almost according to Vegards law
- X at 33.3% Nb and Y at 33.3% Ta would match lattice constant of MgB_2

References

1. Y. Shang et al. Scripta Materialia 240 (2024) 115837; J. Alloy. Compd. 440 (1–2) (2007) L18–L21.
2. APL Mater. 1, (2013) 011002; Sci Data 4, (2017) 160134
3. CASM, v1.1.1 (2021). Available from https://github.com/prisms-center/CASMcode

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