Evaluating the Hardness of Yttrium Ruthenium Borides

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High Hardness Materials

High hardness materials are difficult to destroy and exhibit resistance to wear and tear, making them useful in a multitude of applications, ranging from drill bits and saw blades to artificial joint replacement.

High hardness materials are often constructed out of transition metal borides and carbides. Their simplicity makes them easy to produce but limits the ability to tune the mechanical properties through chemical substitution.

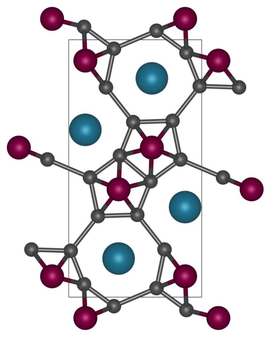
As a result, this work investigates ternary borides that may have high hardness. The focus of this project will be three compounds of the same elements but of different empirical formulas.

Crystal Structures

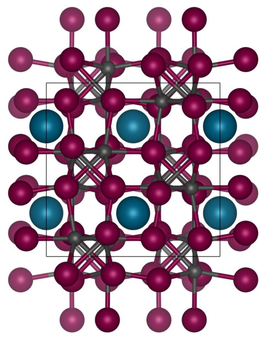
Three yttrium ruthenium borides are reported to exist on the Pearson's Crystal Data: $YRuB_4$, YRu_3B_2, and YRu_4B_4.

The crystal structures of the three yttrium ruthenium borides are very different, despite being composed of the same elements.

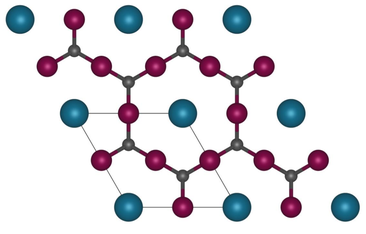
$YRuB_4$

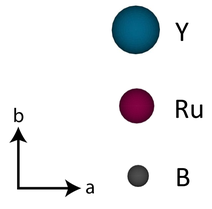


YRu_4B_4



YRu_3B_2

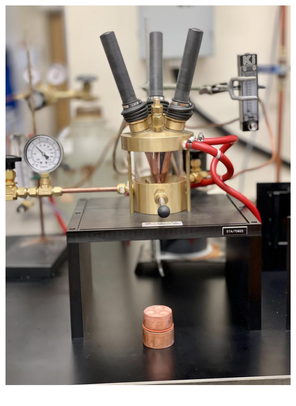




Methods of Synthesis

The yttrium ruthenium borides were synthesized by arc-melting the elemental powders in the desired stoichiometric ratios.

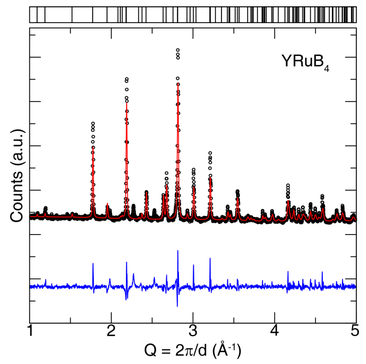
The pellets are loaded into an arc-melter chamber that is filled with argon gas. A high current is applied creating a 3000°C plasma to melt the starting elements.



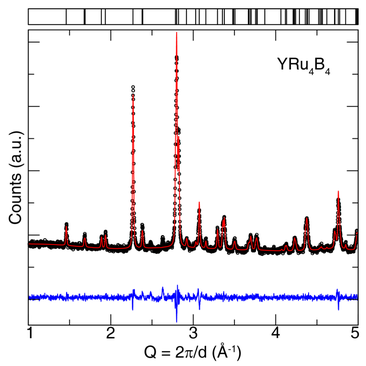
Characterisation of the Samples

The phase purity of three of the samples were characterised by Le Bail refinement of the powder X-ray diffractograms.

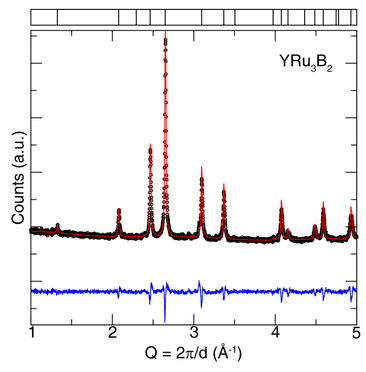
Cell Parameters
Pbam
a = 5.9534 Å
b = 11.5097 Å
c = 3.5452 Å



Cell Parameters
$I4_1/acd$
a = 7.442 Å
b = 7.4420 Å
c = 14.9860 Å

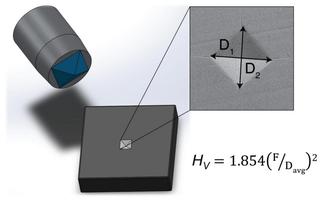


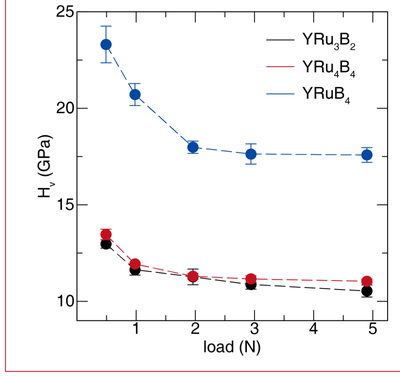
Cell Parameters
P6/mmm
a = 5.4766 Å
b = 5.4766 Å
c = 3.0240 Å



Vickers Microhardness

The Vickers hardness indentation involves indenting the sample with a diamond-tip indenter. The program then reads the diagonals of the indents and provides a value of hardness in gigapascals.





The favoured structure design for hardness is a boron network, as the hardness of $YRuB_4$ is significantly higher than that of the other two compounds.

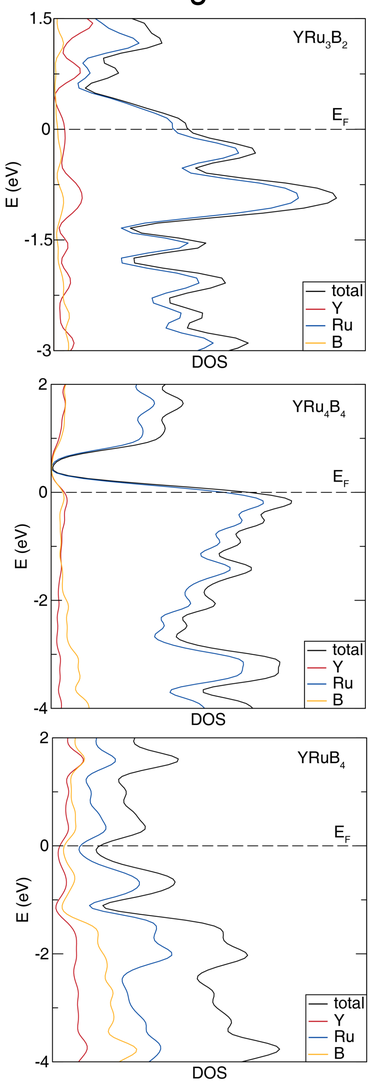
Altering Hardness with Electronic Tuning

The density of states curves indicate where the Fermi level lies.

Different metals may substitute into a structure to alter the electron count, modulating the Fermi level.

The energetically favourable position for the Fermi level is in a pseudogap, increasing the stability of the phase and enhancing mechanical properties.

This design concept is nonspecific and can be applied to other systems where fermi level position can act a proxy to potentially increase experimental hardness.



Conclusions and Future Work

In conclusion, the yttrium ruthenium tetraboride exhibits high hardness. This work also highlights the desired boron networks and energetic stability that enhances the hardness of intermetallic borides.

Future work would involve substitution of the yttrium or ruthenium with another metal to reduce the electron count. The Fermi level shift further into the pseudogap ideally should enhance hardness.

Acknowledgements

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References

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