Ab initio predicted micro-mechanical performance of refractory high-entropy alloys

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Recently developed high-entropy alloys (HEAs) consisting of multiple principal elements represent a new field of metallurgy and have demonstrated appealing properties for a wide range of applications. Using *ab initio* alloy theory, we reveal the alloying effect on the elastic properties and the ideal tensile strength (ITS) in the [001] direction of four body-centered cubic (bcc) refractory HEAs based on Zr, V, Ti, Nb, and Hf. We find that these HEAs show high elastic anisotropy and large positive Cauchy pressure, suggesting good extrinsic ductility. Starting from ZrNbHf, it is found that the ITS decreases with equimolar Ti addition. On the other hand, if both Ti and V are added to ZrNbHf, the ITS is enhanced by about 42 %. An even more captivating effect is the ITS increase by about 170 %, if Ti and V are substituted for Hf. The alloying effect on the ITS is explained by the d-band filling. A brittle-to-ductile transition is found in terms of the failure-mode under uniaxial tension. These investigations suggest that intrinsically ductile HEAs with high ideal strength can be achieved by controlling the proportion of group four elements to group five elements.âĂŃ

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