MIXING THE TRANSITION METALS IN TRANSITION METAL CARBIDES

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One avenue of developing new ultrahigh temperature ceramics is through the use of multiple principal component ceramics. These so-called high entropy ceramics are similar to high entropy alloys and have the potential to exhibit superior properties as compared materials with fewer elements, e.g. $TaHfZrTiC_4$ compared to TiC. However, the cause of mixing, be it enthalpy or entropy, and the thermodynamic stability of these compounds is not well known. Here, we investigate the thermodynamics of mixing multiple principal elements in the transition metal carbides from binary solutions to 7 element transition metal solutions using a combination of density functional theory and computational thermodynamics. We find that while increasing the number of elements increases solubility of the solution in a general sense, this is not a universal trend and depends strongly on the types of transition metals in the solution. Furthermore, we demonstrate that many multiple principal element transition metal carbides are not stable below 1000°C. These results provide direct insight into the stability of thye solutions, and which transiton elements will increase solubility and therefore stability.

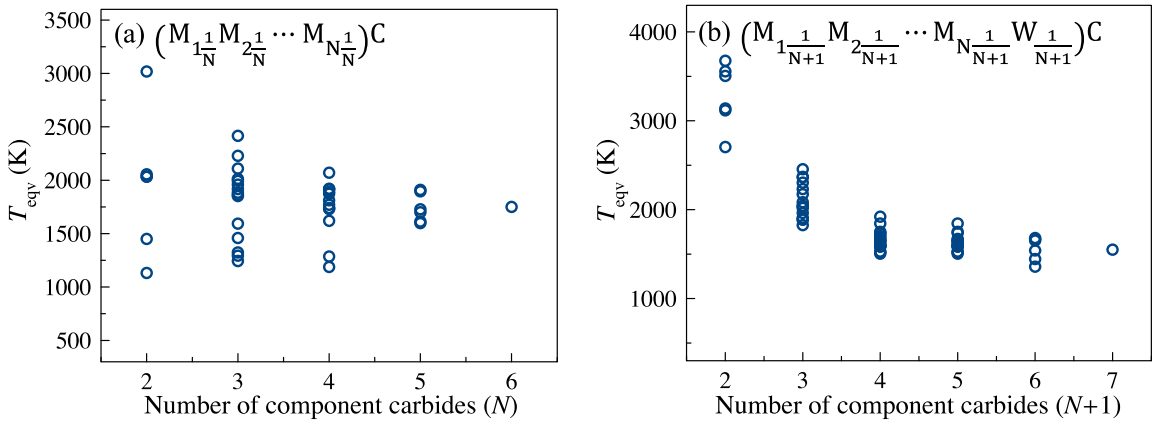

Figure 1: The minimum equilibrium temperature for equiatomic multiple transition element carbide solutions as a function of temperature (a) with and (b) without tungsten.