HfNbTaTiZr complex concentrated alloys, their microstructure and positron characteristics

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Studying complex concentrated alloys (CCAs; also often called high entropy alloys) [1] is very popular at present. The equiatomic, refractory alloy HfNbTaTiZr [2] belongs to this class and was devised for high temperature and biocompatible applications. This alloy exhibits the bcc structure at high temperatures due to the fact that all constituting elements show the bcc structure at such temperatures, and have very similar metallic radii (and thus easily mix). High configurational entropy is not needed to explain single, bcc phase of HfNbTaTiZr at high temperatures (even if high entropy contributes to the alloy stability, as does the mixing enthalpy). Upon cooling, there is a strong tendency to local order [3], which lowers the entropy, and eventually the alloy separates into two, hcp and bcc, phases with non-equiatomic compositions [4].

Since the understanding of any material has to rely on its microstructure, we proceed in this direction and simulate various structure-related properties of the HfNbTaTiZr alloy. An attempt is undertaken to simulate phase separated HfNbTaTiZr system, following the idea of phase transition in ZrNb alloys where the transition from bcc to hcp phase occurs when cooled [5], using the general geometrical relationship of these two phases [4,6]. It is also explained why the studied alloy cannot have a single, hcp structure, which might look natural since Hf, Nb, and Zr (making thus atomically 60 % of the alloy) are hexagonal (hcp) at low temperatures. In the simulations a pseudopotential code based on the density functional theory was employed.

Positron characteristics, such as the lifetime and affinity, of various alloys' configurations were also calculated, and we discuss what is possible to deduce from them in relation to the microstructure of the studied alloy. The role of unintentional impurities, like oxygen and nitrogen, is also examined.

References

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