AB-INITIO MODELING AND EXPERIMENTAL INVESTIGATION OF THE PROPERTIES OF ULTRA-HIGH TEMPERATURE SOLID SOLUTIONS $Ta_xZr_{1-x}C$

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Due to their high melting temperature, resistance towards high-temperature oxidation and high mechanical properties, solid solutions $Ta_xZr_{1-x}C$ are promising carbides for the application as the ultra-high temperature materials (UHTCs).

The absence of reliable data on the phase equilibria in the Ta–Zr–C system hinders the development and implementation of the related UHTCs. In particular, there are contradictory reports regarding the existence of the miscibility gap in Ta–Zr–C system at the temperatures lower than 900 ^{o}C [1–3].

In this work, we carry out ab-initio calculation of the thermodynamic properties of $Ta_xZr_{1-x}C$ alloys and demonstrate that the decomposition of the solid solutions into TaC and ZrC should not occur.

Among the various methods that allow the synthesis of solid solution in Ta–Zr–C system, self-propagating high-temperature synthesis is widely considered one of the most prospective [4, 5].

We synthesize single-phase specimens with the composition $Ta_xZr_{1-x}C$ (x=0.9, 0.8, 0.6, 0.3) and anneal it for 40 hours. We do not observe any sign of the decomposition of the solid solution during the annealing, corroborating the conclusions obtained in theoretical simulations.

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