On the stoichiometry of zirconium carbide

Claudia Gasparrini, Dhan-sham Rana, Niccolò Le Brun, Denis Horlait, Christos N. Markides , Ian Farnan, William e. Lee

Scientific Reports (2020) 10:6347 https://doi.org/10.1038/s41598-020-63037-0

Abstract:

The dependencies of the enhanced thermomechanical properties of zirconium carbide (ZrCx) with sample purity and stoichiometry are still not understood due to discrepancies in the literature. Multiple researchers have recently reported a linear relation between the carbon to zirconium atomic ratio (C/Zr) and the lattice parameter, in contrast with a more established relationship that suggests that the lattice parameter value attains a maximum value at a C/Zr similar to 0.83. In this study, the relationship between C/Zr atomic ratio and the lattice parameter is critically assessed: it is found that recent studies reporting the thermophysical properties of ZrCx have unintentionally produced and characterised samples containing zirconium oxycarbide. To avoid such erroneous characterization of ZrCx thermophysical properties in the future, we propose a method for the accurate measurement of the stoichiometry of ZrCx using three independent experimental techniques, namely: elemental analysis, thermogravimetric analysis and nuclear magnetic resonance spectroscopy. Although a large scatter in the results (Delta C/Zr = 0.07) from these different techniques was found when used independently, when combining the techniques together consistent values of x in ZrCx were obtained.