High-entropy alloys for high-pressure hydrides

Felipe Marques, Michael Felderhoff

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

e-mail: fmarques@kofo.mpg.de

Recently, high-entropy alloys (HEAs), started to be investigated for their hydrogen storage properties. In terms of materials for hydrogen storage, the vast compositional domain presented by HEAs with the formation of simple crystalline structures has indicated new possibilities for adjusting the properties of hydrides. HEAs have presented improved properties, such as increased gravimetric capacity at moderate conditions and complete storage reversibility at room temperature without activation processes. [1] Nonetheless, it is worth pointing out that the focus of the investigation of HEAs for hydrogen storage has been only on alloys systems that may store hydrogen under moderate conditions of pressure (< 10 MPa). Alloy systems (especially intermetallic forming ones) that are capable of storing hydrogen reversibly under medium to high pressures (> 10 MPa) have already been reported. The hydrides formed under these conditions could be used in applications, such as hydrogen compression and hybrid hydrogen storage tanks (combining hydrides with compressed hydrogen).[2] In this regard, the investigation of intermetallic HEA systems that may form medium to high-pressure hydrides can be promising.

In this work, we designed a HEA composition by using the CAlculated PHAse Diagram (CALPHAD) method and synthesized it via the arc melting technique. According to the design, the AB_2 HEA composition, in which the A elements selected were Ti and Zr, and the B elements were Cr, Fe, and Al, should, after synthesis, present a structure composed mainly of C14 Laves phase (P36/mmc). The $TiZrAl_{1.33}Cr_{1.33}Fe_{1.33}$ composition was synthesized and submitted to a heat treatment (HT) after synthesis (400 °C for 4.5 h in a TG/DSC). Characterization via Powder XRD and SEM-EDX indicated that after synthesis a single C14 Laves phase was present and this phase was stable up to 400 °C (no phase decomposition after HT). Pressure-composition-isotherms (PCIs) recorded for a sample of this material showed absorption of approximately 1.9 wt.% H_2 (H/M = 1) at 100 °C up to 15 MPa. The shape of the isotherms indicated absorption via solid solution only, without any defined plateau pressure under the conditions tested. These results may call attention to a new promising field of investigations of HEAs for hydrogen storage.

References

1. Marques, F., Balcerzak, M., Winkelmann, F., Zepon, G. & Felderhoff, M. Review and outlook on high-entropy alloys for hydrogen storage. Energy & Environmental Science 14, 5191-5227 (2021).
2. Cao, Z. et al. Development of ZrFeV alloys for hybrid hydrogen storage system. International Journal of Hydrogen Energy 41, 11242-11253 (2016).

Felipe Marques received his M.S. degree in Materials Science and Engineering from the Federal University of São Carlos (UFSCar), Brazil in 2020. He is currently a Ph.D. student in the Department of Heterogeneous Catalysis at Max-Planck-Institut für Kohlenforschung, Germany. His current research activities are focused on the design, synthesis, and characterization of high-entropy alloys for hydrogen storage and high-pressure metal hydrides for hybrid hydrogen storage systems.