Investigation of high temperature properties of BCC hydrogen storage alloys

Abstract:

The energy demands for the applications and the developing energy systems must be practical, cost-effective, sustainable, reliable and should have a very low impact on the environment. As of now, fossil fuels are being widely used for the energy systems and transportation all over the world. However, the burning of fossil fuel releases a high amount of $CO₂$ emission which is polluting the air and making global warming. As a solution to this problem, the hydrogen energy technology can be an efficient and suitable technology for the on-board vehicular applications. The development of hydrogen storage material is very important for establishing hydrogen energy infrastructure all over the world in near future. Particularly, the hydrogen storage materials should possess high hydrogen capacity with moderate thermodynamic properties as well as optimum kinetics. Recently, the development of metal hydride compressor is a promising technology for hydrogen compression which has the capability of compressing hydrogen to a high pressure by only increasing heat without the need of any moving mechanical parts.

In this thesis, the hydrogen storage properties and the compressor cyclic performance of V-Ti-Cr BCC alloys were systematically investigated to understand the effect of high temperature and pressure conditions on their sorption performance.

 $V_{20}Ti_{32}Cr_{48}$ and $V_{40}Ti_{21.5}Cr_{38.5}$ two different composition alloys were selected for this study according to their effective hydrogen storage performance. The hydrogen sorption capacity of high vanadium content $V_{40}Ti_{21.5}Cr_{38.5}$ alloy is stable after 10 cycles with their plateau pressures and hysteresis remain almost the same up to 100 cycles. Whereas, low vanadium content $V_{20}Ti_{32}Cr_{48}$ alloy continuously degraded in terms of their hydrogen storage capacity over a number of cycles. Structural and morphological investigations suggest that the low vanadium content alloy have two stable hydride phases i.e $TiH_{0.66}$ and $VH_{0.81}$ after compressor cycling, which requires more than 400 $^{\circ}$ C to desorb hydrogen completely. This seems to be the responsible reason for the hydrogen storage capacity decrease in each successive cycle of the $V_{20}Ti_{32}Cr_{48}$ alloy.

In order to improve the cyclic and hydrogen storage properties of $V_{40}Ti_{21.5}Cr_{38.5}$ alloy further, the fourth element has been substituted for Cr. Niobium, Iron, and Zirconium elements were selected to alter the thermal stability as well as the

cyclic performance of $V_{40}Ti_{21.5}Cr_{38.5}$ ternary alloy at moderate conditions. The $V_{40}Ti_{21}$, Cr_{33} , Nb_5 alloy was found stable after 50 cycles of compressor cyclic test with a higher hydrogen sorption capacity than that of parent and other two alloys. Structural and morphological investigations suggest the formation of $VH_{0.81}$ phase responsible for initial capacity decay for Nb substituted alloy which could not desorb hydrogen at the studied temperature range. The Fe doped $V_{40}Ti_{21.5}Cr_{33.5}Fe_5$ alloy was found continuously degraded over a number of cycles with hydrogen storage capacity. However, structural and morphological investigations suggest no phase segregation during the cycling of $V_{40}Ti_{21.5}Cr_{33.5}Fe_5$ alloy in contrast to the other alloys, which suggest that phase segregation is not the only responsible reason for the performance degradation of BCC alloys employed for compressor cycle. In some cases similar to $V_{40}Ti_{21.5}Cr_{33.5}Fe_5$, stress/strain formation in the lattice during cycling may also cause the degradation of the material. On the other hand, the hydrogen sorption capacity of Zr doped $V_{40}Ti_{21.5}Cr_{33.5}Zr_5$ alloy was found stable after 25 cycles with its plateau pressures and hysteresis remain same up to 100 cycles. The initial degradation was suggested to be associated with the formation of stable hydride phases ZrV_2H_x .