# COMPOSITION EFFECT ON THE HYDROGEN ABSORPTION PROPERTIES OF REFRACTORY HIGH ENTROPY ALLOYS

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Among various materials for solid-state hydrogen storage, alloys and intermetallics forming hydrides are one of the most important classes due to their high-volume density, reversibility, and safety [1]. Recently, a new metallurgy paradigm of alloying has emerged based on the concept of high entropy alloys (HEAs), initially intended to enhance the mechanical properties [2]. The principle is laid on the mixing of elements close to the equimolar proportion for systems up to five and more elements. This may lead to the formation of simple single-phased solid solutions (bcc, fcc and hcp) with interesting properties for solid-sate hydrogen storage. We will focus here on the physicochemical and the hydrogen absorption/desorption properties of a series of HEAs $(Ti\text{-}V\text{-}Zr\text{-}Nb)_{90}X_{10}$ (with $X$ = Mg, Al, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo and Ta) and the insights that can be obtained from experiments at large-scale facilities, mainly neutron and X-ray diffraction. The role of additional element $X$ will be highlighted and compared to the quaternary pristine Ti-V-Zr-Nb alloy as function of local lattice distortion and electronic properties [3–5]. For example, *in situ* neutron diffraction at D1B ILL has clearly evidenced a drastic decrease of the desorption temperature associated with the phase transition from a fcc hydride to a bcc alloy in the Al-containing material as compared to the initial quaternary composition [6]. This approach is envisioned to clarify the role of the chemical composition on the hydrogen storage performances of refractory HEAs.

References

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|  | CZ research interests focus on the synthesis and the characterisation of materials for solid-state hydrogen storage by combining laboratory and large-scale facilities. She is currently studying both nano- and bulk-like materials: nanocomposites (metal nanoparticles inserted into porous hosts and single atoms dispersed on porous carbons) to highlight the nanoscale effects on the hydrogen ad/absorption properties and bulk high entropy alloys to clarify the role of the chemical composition on the hydrogen absorption performances. |