Non-Equilibrium Manufacturing of Nanostructured Complex Metal Hydrides for Solid State Hydrogen Storage

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Abstract: Hydrogen as an important potential energy vector in the energy transition has been considered as an alternative fuel and studied in past decades targeting mid-term decarbonizing opportunities. For hydrogen to become a viable energy carrier, advanced hydrogen storage materials will be required, which is the major challenging issue that cuts the distribution, and safe end-uses of hydrogen as a fuel. More compact, low weight, low cost, safe, and efficient storage materials and systems operating at near room temperature at low pressure are essentially required that can satisfy all the required targets set by the US Department of Energy. We are targeting the integrated computational and experimental framework for the design and manufacturing of nanostructured complex metal hydrides, particularly with perovskite structure, by non-equilibrium approach. This framework consists of three major components: 1) Computational data generation through high throughput first-principles calculations based on the density functional theory (DFT) and CALculation of PHAse Diagrams (CALPHAD) modeling of phase stability; 2) Advanced manufacturing techniques utilizing arc melting/induction melting, non-equilibrium melting spinning (MS) and high energy ball milling; 3) Systematic characterization to investigate the underlying mechanism of the materials in terms of phase formation and transition, microstructure, hydrogen storage capacity and absorption/desorption kinetics. Our current research has designed and developed several perovskite-type complex metal hydrides with a potential hydrogen content up to ~15% and a moderate hydrogen release temperature of up to 400 °C. These findings depict the advantage in high hydrogen storage capability compared to conventional metal hydrides and in mild operational condition compared to compressed and liquid hydrogen. The results can potentially provide more efficient and safer hydrogen storage solutions towards viable energy carriers for sustainability.