8P55

先進的中性子増倍材開発に向けたベリリウム金属間化合物の電子的記述子の探索

Electronic descriptor of Be intermetallics for the development of advanced neutron multiplier

向井啓祐[1)]、笠田竜太[2)]、金宰煥[3)]、中道勝[3)]
Keisuke MUKAI, Ryuta KASADA, Jae-Hwan KIM, Masaru NAKAMICHI

(1)京大、2)東北大、3)量研機構)
(1) Kyoto University, (2) Tohoku University, (3) QST

Be-rich beryllides have attracted increasing attention as neutron multipliers for nuclear fusion reactors as a substitute for pure Be metal, because the low chemical reactivity with steam can significantly reduce hydrogen generation by two orders of magnitude in a loss-of-coolant accident. The Be compound is used to multiply neutrons via the ^{9}Be(n,2n) reaction in a fusion breeding blanket to ensure fuel self-sufficiency; hence, a beryllide with a high Be atomic density, reduced retention characteristics of hydrogen isotopes, and minimum radio-activation is desired. Nevertheless, such developments of beryllide neutron multipliers have been limited not only by the toxicity of Be dust in manufacturing process, but also by time-consuming and expensive neutron irradiation tests performed using research reactors.

First-principles calculations were systematically carried out on 42 existing binary beryllides to find an effective electronic descriptor which helps to search favorable Be-rich intermetallics. Vacancy formation energy of Be atom and hydrogen solution energy were chosen as measures for defect formation and hydrogen retention properties, respectively.

Density functional theory (DFT) calculations were performed using the revised Perdew−Burke−Ernzerhof (RPBE) generalized gradient approximation for the exchange and correlation functional implemented in the Vienna ab initio simulation package (VASP). The valence band was experimentally investigated by using soft X-ray emission spectrometer (SXES) attached to a JXA-8500F field-emission electron probe micro-analyzer (EPMA) by JEOL.

Figure 1 shows the Be atomic density plotted with averaged Be vacancy formation energy in Be metal and intermetallics. Although the Be atomic densities decreased by the formation of intermetallic phases, most of the Be intermetallics exhibited higher Be vacancy formation energies than the Be metal, except for $Be_{12}X$ with X being the late transition metals (TMs: X = Co, Pd, Pt, Ag, and Au). In the presentation, an effective electronic descriptor for vacancy energy and hydrogen solution energy will be reported.

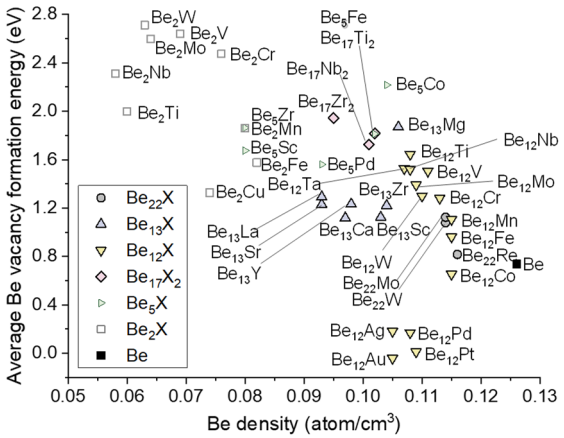

Figure 1. Plot of Be atomic density with average Be vacancy formation energy of the Be metal and intermetallic compounds.