05,07

First-Principles Study of the Physical Properties of the New Quaternary Heusler Alloy CoMnVZ (Z = Sn and Sb)

© H.-J. Zhou, H.-M. Huang¶, S.-J. Luo

School of Science, Hubei University of Automotive Technology,
Shiyan, China

¶ E-mail: smilehhm@163.com

Received: August 10, 2020
Revised: August 14, 2020
Accepted: August 20, 2020

The physical properties of two new quaternary Heusler alloys CoMnVSn and CoMnVSb were systematically studied by using first-principles calculation. The results show that the type-1 structures of ferromagnetic phase for these two alloys are the most stable. They all exhibit half-metallic behavior at equilibrium, and their half-metallic characteristics are maintained in the lattice region of 5.73−6.19 Å for CoMnVSn and 5.82−6.18 Å for CoMnVSb. The calculated magnetic moment Mt of each molecular unit in the half-metal lattice region strictly follows the Slater–Pauling empirical rule $M_t = Z_t - 24$, where Z_t is the number of valence electrons. The elastic constants show that the mechanical properties of the two compounds are stable at equilibrium, and the anisotropy factor and three-dimensional Young's modulus confirm that they have anisotropy. It is expected that the CoMnVSn and CoMnVSb alloys are promising candidates in spintronics.

Keywords: quaternary Heusler alloy, electronic structure, half-metal, first principles.