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Thermoelectric properties, phonon, and mechanical stability of new half-metallic quaternary Heusler alloys: FeRhCrZ (Z = Si and Ge)

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ABSTRACT

Computer simulations within the framework of density functional theory are performed to study the electronic, dynamic, elastic, magnetic, and thermoelectric properties of a newly synthesized FeRhCrGe alloy and a theoretically predicted FeRhCrSi alloy. From the electronic structure simulations, both FeRhCrZ (Z = Si and Ge) alloys at their equilibrium lattice constants exhibit half-metallic ferromagnetism, which is established from the total magnetic moment of 3.00 μB, and that the spin moment of FeRhCrGe is close to the experimental value (2.90 μB). Their strength and stability with respect to external pressures are determined by simulated elastic constants. The Debye temperatures of FeRhCrSi and FeRhCrGe alloys are predicted to be 438 K and 640 K, respectively, based on elastic and thermal studies. The large power factors (PFs) of the two investigated alloys are in contour with those of the previously reported Heusler compounds. Besides, the conservative estimate of relaxation time speculated from the experimental conductivity value is 0.5×10^{-15} s. The room temperature PF values of FeRhCrSi and FeRhCrGe compounds are 2.3 μW/cm K^2 and 0.83 μW/m K^2, respectively. Present investigations certainly allow the narrow bandgap, spin polarization, and high PF values to be looked upon for suitable applications in thermoelectrics and spintronics.

INTRODUCTION

Exploration of new materials, particularly the Heusler alloys and their offshoots accompanied by tunable properties, has attained significant attention from the material scientists worldwide. Modern technologies ranging from superconductivity to energy conversion and data storage to contactless sensing are typically boosted by Heusler alloys. This class of materials emerged as the ground-breaking area of research due to multi-dimensional properties like compatible thin film interfaces, large Curie temperatures, magnetoresistance, etc.[1,2] The scientific community accomplished sufficient research for the prediction of new materials with some predefined properties such as half-metallicity, high spin polarization, or large integral magnetic moments. Half-metallic ferromagnets (HMFs) represent a new class of materials that exhibit semiconducting properties in one spin (down) channel and behave as a conductor in the other spin (up) channel. They find applications in spintronics for developing basic computer units, data storage devices, magnetic sensors, high-tech electronic devices, spin valves, and tunnel junctions. The phenomenon of half-metallicity in Heusler alloys was first predicted by Groot *et al.* in 1983.[3–5] For several years, great effort was put forth to study the HMF character originating from the *d*-orbitals of transition elements in such materials. Until today, five kinds of HMFs have been anticipated: the oxide compounds such as CrO_2,[6] TiO_2, and VO_2,[7] some ternary compounds (specifically, spinels with the general formula AB_2O_4 such as Fe_3O_4 and $LiMn_2O_4$[8–10]), single or double perovskites (e.g., $BaPaO_3$ and Sr_2SnMnO_6[11,12]), and dilute magnetic semiconductors [DMSs, e.g., Cu-doped ZnO,[13] Cr-doped CdZ (Z = S, Se, and Te),[14] Mn-doped GaN,[15] etc.]. In addition, the Heusler materials that include half Heuslers [e.g., CoCrZ (Z = S and Se)],[16] full Heuslers [Co_2TaZ (Z = Si and Ge)],[17] and quaternary Heuslers (FeVRuSi[18]) have also accounted for the integral magnetic moment, spin polarization, and half-metallic properties.