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PAPER

Tailoring the physical characteristics of novel quaternary RuMnCrSi and NiMnCrAl compounds for spintronic and thermoelectric applications

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Abstract

In the development of advanced magneto-electronic systems, materials with high spin polarization are essential for optimizing device performance. This research explores the elastic, optical, electronic, magnetic, and thermoelectric characteristics of the Heusler alloys RuMnCrSi and NiMnCrAl. Through density functional theory (DFT) simulations, we determine that RuMnCrSi adopts a Type III crystal structure, while NiMnCrAl exhibits a Type I structure. Both structures correspond to the most stable phases for the respective alloys. The electronic properties reveal that both compounds exhibit half-metallic ferrimagnetic behavior, with RuMnCrSi showing a band gap of 0.806 eV in the majority spin channel and NiMnCrAl presenting a metallic character with no gap in the majority spin channel. The calculated total magnetic moments for RuMnCrSi and NiMnCrAl are 2 $\mu\beta$ and 1 $\mu\beta$, respectively, confirming their ferrimagnetic half-metallic nature and 100% spin polarization. Elastic constant calculations confirm the mechanical stability of both alloys, supporting their potential for practical applications. The optical properties, including the dielectric function, absorption, reflectance, and optical conductivity, were also analyzed. Both alloys demonstrate strong ultraviolet (UV) absorption, with high refractive indices, suggesting their suitability for use in spintronic devices and UV photodetectors. In the thermoelectric evaluation at 900 K, NiMnCrAl and RuMnCrSi exhibit promising performance, with ZT values of 0.3004 and 0.1977 under p-type conditions, respectively. These ZT values significantly increase to 0.6101 and 0.3583 under n-type conditions. The optimal carrier concentrations for NiMnCrAl and RuMnCrSi in p-type conditions are 0.1849×10^{20} cm^{-3} and 0.1290×10^{20} cm^{-3}, and in n-type conditions, they are -0.1421×10^{20} cm^{-3} and -0.1688×10^{20} cm^{-3}, respectively. These findings highlight the remarkable potential of RuMnCrSi and NiMnCrAl alloys in thermoelectric and spintronic applications, offering a promising avenue for next-generation energy-efficient materials and devices.

1. Introduction

Since the publication by de Groot *et al* regarding the prediction of half-metallicity in NiMnSb [1], the investigation of Heusler compounds has emerged as a prominent field of research. This specific characteristic holds potential for enhancing the efficiency of spintronics devices. Half-metals are defined as substances in which the electrons in two separate spin channels demonstrate diametrically opposed properties, thereby permitting complete spin polarisation in the vicinity of the *Fermi* level. By leveraging both charge and spin, these substances demonstrate tremendous promise for spintronics by enabling the manipulation of data storage capacity, device configuration, volatility, and dimensions. The exponential advancements in scientific research and technology have enabled the development of innovative materials with a wide range of functionalities. However, the practical implementation of these materials in spintronics technology systems is impeded by a