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Electronic, magnetic and thermal properties of $Co_2Cr_xFe_{1-x}X$ (X=Al, Si) Heusler alloys: First-principles calculations

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ABSTRACT

Density functional theory (DFT) based on the full-potential linearized augmented plane wave (FP-LAPW) method is used to investigate the structural, electronic, magnetic and thermal properties of $Co_2Cr_xFe_{1-x}X$ (X=Al, Si) full Heusler alloys, with $L2_1$ structure. The structural properties and spin magnetic moments are investigated by the generalized gradient approximations (GGA) minimizing the total energy. For band structure calculations, GGA, the Engel–Vosko generalized gradient approximation (EVGGA) and modified Becke–Johnson (mBJ) schemes are used. Results of density of states (DOS) and band structures show that these alloys are half-metallic ferromagnets (HMFS). A regular-solution model has been used to investigate the thermodynamic stability of the compounds $Co_2Cr_xFe_{1-x}X$ that indicates a phase miscibility gap. The thermal effects using the quasi-harmonic Debye model are investigated within the lattice vibrations. The temperature and pressure effects on the heat capacities, Debye temperatures and entropy are determined from the non-equilibrium Gibbs functions.

1. Introduction

Since de Groot et al. [1] have discovered the half-metallic ferromagnetism in NiMnSb semi-Heusler compound using first principle calculations based on density functional theory, many other experimental and theoretical studies were focused on the Heusler alloys due to the need of a high spin polarized ferromagnetic compound with a high Curie temperature, These studies can contribute to the rapid development of spintronics applications. The Half-Heusler alloys have the formula XYZ and are ordered in $C1_b$-type.The full Heusler alloys are ternary intermetallics ferromagnetic compounds with the formula X_2YZ and are ordered in the $L2_1$-type face centered cubic structure, usually made from non-ferromagnetic constituents, two transition metals (X, Y) and a main group element (Z). The Half-metallic compounds are characterized by the conducting majority states but the semiconducting minority states. Co_2-based compounds are very promising for spintronic applications due to their three special properties, Curie temperature, spin polarization and magnetic moment. They were investigated theoretically and most of them were predicted to be half-metallic using ab-initio calculations. The large variety of possible compositions of the Heusler compounds allows one to easily produce materials with predictable magnetic properties. The prediction of new materials could be done by the exchange of the elements X, Y, and Z [2,3]. Among the Heusler compounds, Co_2XY are especially promising materials for spintronics applications due to their wide band gap in the minority spin states and are easy to be synthesized [4,5]. Co-based Heusler alloys were investigated theoretically using ab initio calculations and most of them are predicted to be half-metallic (HM) [6,7]. With the desire of finding new promising half metals, the Co_2YSi series was also explored by many theoreticians [8,9].

The Co_2YZ (Y=Cr, Fe; Z=Si, Al) compounds were studied by several groups. Aly and Shabara [10] showed that the energy gap-pressure dependence of Co_2CrSi exhibits half-metallicity in the pressure range 0–150 GPa with a some what weak pressure-dependence.Wurmehl et al. [11] studied the Co_2FeSi compound showing that it is a half-metallic ferromagnetic compound with a high Curie temperature and magnetic moment.

The substitution of Fe atom instead of Cr atom in the Co_2CrX (X=Si,Al) alloys was studied by many researchers [12–14]. Despite the many investigations on this doped type of alloy, looking at it

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Table 1
Calculated lattice parameter (a) and bulk modulus (B) for $Co_2Cr_xFe_{1-x}Al$ and $Co_2Cr_xFe_{1-x}Si$ alloys for various x compositions.

Alloys	x	Lattice constant a (Å) GGA			Bulk modulus B (GPa)		
		This work	Experiment	Other works	This work	Experiment	Other works
$Co_2Cr_xFe_{1-x}Al$	0	5.706	5.73[a], 5.727[b]	5.692[c], 5.69[d]	188		210[a], 207.23[d]
	0.25	5.706			194		
	0.5	5.706			197		
	0.75	5.708			199		
	1	5.711	5.73[a], 5.727[b]	5.708[c] 5.70[d]	192		217[a], 215.87[d]
$Co_2Cr_xFe_{1-x}Si$	0	5.634	5.64[e]; 5.636[f]	5.618[g]; 5.63[i]	203	240[h]	207.1[g], 204[j]
	0.25	5.643		5.64[k]	210		
	0.5	5.644		5.64[k]	216		
	0.75	5.645		5.64[k]	220		
	1	5.645	5.65[l]	5.634[m]; 5.6[n]	224		239[m]; 227[l]

[a] Ref. [12].
[b] Ref. [13].
[c] Ref. [6].
[d] Ref. [27].
[e] Ref. [11].
[f] Ref. [31].
[g] Ref. [29].
[h] Ref. [32].
[i] Ref. [30].
[j] Ref. [8].
[k] Ref. [14].
[l] Ref. [5].
[m] Ref. [28].
[n] Ref. [10].

Table 2
Calculated total and partial magnetic moments m_s (μ_B) for $Co_2Cr_xFe_{1-x}Al$ and $Co_2Cr_xFe_{1-x}Si$ alloys for various x compositions.

	x	m_s (μ_B)										
		This work										Otherworks
		TOT		Co		Al		Cr		Fe		TOT
		GGA	MBJ	GGA	MBJ	GGA	MBJ	GGA	MBJ	GGA	MBJ	
$Co_2Cr_xFe_{1-x}Al$	0	4.89	5.00	1.22	1.37	−0.01	−0.05			2.62	2.84	4.96 [6]
	0.25	4.50	4.50	1.12	1.24	−0.05	−0.10	1.61	1.52	2.77	2.84	
	0.5	4.01	4.00	1.03	1.17	−0.05	−0.10	1.53	1.42	2.78	2.83	
	0.75	3.50	3.50	0.92	1.01	−0.05	−0.09	1.49	1.36	2.79	2.85	
	1	2.99	3.00	0.82	1.03	−0.03	−0.04	1.39	1.27			2.98 [12]
$Co_2Cr_xFe_{1-x}Si$	x	TOT		Co		Si		Cr		Fe		
	0	5.47	5.84	1.37	1.54	−0.003	−0.002			2.75	2.96	5.97 [35] 5.48 [8]
	0.25	5.33	5.49	1.33	1.44	−0.03	−0.02	2.25	2.35	2.90	3.00	
	0.5	4.95	5.00	1.22	1.33	−0.001	−0.022	2.18	2.21	2.92	2.98	
	0.75	4.50	4.50	1.12	1.22	−0.05	−0.05	2.10	2.06	2.90	2.94	
	1	4.00	4.00	1.02	1.13	−0.03	−0.04	1.85	1.85			4.00 [10] 4.00 [8]

from different perspectives, there are still many properties which need to be explored to gain insight. We focus in this work on the thermodynamic and thermal properties. We have investigated the $Co_2Cr_xFe_{1-x}X$ (X=Al, Si) full Heusler alloys by using the full potential linear augmented plane wave (FPLAPW) method within the generalized gradient approximation (GGA), Engel Vosko Generalized Gradient Approximation (EVGGA) and the modified Becke Johnson approximation (mBJ) in order to study the structural, electronic, magnetic and thermal properties.

2. Computational details

The calculations were done using the scalar relativistic full potential linearized augmented plane wave FP-LAPW+lo method [15–17] within the DFT [18,19] as included in the WIEN2k [20] code. Structural properties were calculated using the generalized gradient approximation (GGA) [21]. In addition, for the electronic properties, we also applied the Engel–Vosko (EVGGA) [22] and modified Becke–Johnson (mBJ) [23] schemes, where the last one is