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Structural and Magnetic Properties of the Mn₅₀Al₄₆Ni₄ Alloy

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Abstract: In this study we present the results of electronic structure calculations and the experimental investigations on the structural and magnetic properties of the $Mn_{50}AI_{46}M_4$ (M = Mn, Ni, Ti) alloys. The highest magnetic moment was found for the $Mn_{50}AI_{46}Ni_4$ alloy. Total energy calculations point to a more stable antiferromagnetic configuration of the Mn^{1a} - Mn^{2e} pair. DTA measurements pointed out the formation of the metastable τ phase around 470 °C and its decomposition into the stable γ_2 and β -Mn(AI) phases at 850 °C. The τ phase was found along with the ϵ' phase only in the as-cast sample and the ones annealed at 470 °C for 6 h. The close values of the theoretical and experimental effective magnetic moments confirm the existence of the ϵ' and τ phases in these alloys.

Experimental and Computational Details:

- Electronic structure calculations were performed in the framework of the Local Density Approximation (LDA) of the Density Functional Theory by means of the SPR-KKR method using the experimentally determined lattice parameters for Mn₅₄Al₄₆ (a = 3.94 Å, c = 3.58 Å). All relativistic effects have been taken into account, including the spin-orbit coupling, in the ferromagnetic (FM) and antiferromagnetic (AFM) spin configurations of the Mn^{1a}-Mn^{2e} pair.
- > The Mn₅₄Al₄₆ and Mn₅₀Al₄₆Ni₄ ingots were prepared by induction melting of the starting components under a purified Ar atmosphere.
- > The samples were annealed in an inert Ar atmosphere at temperatures between 470 and 850 °C for different times followed by quenching in water.
- > XRD investigations were performed using a Brüker D8 Advance X-ray diffractometer with Cu K_{α} radiation.
- Differential thermal analysis (DTA) was performed between 100 and 900 °C under Ar atmosphere with a temperature ramp rate of 20 °C/min.
- The magnetization and magnetic susceptibility were measured with a Weiss-type magnetic balance in a temperature range of 300-800 K.

Electronic Structure Calculation Results:

Calculated magnetic moments for the τ phase of Mn₅₀Al₄₆ M_4 (M = Ni, Ti), Mn₅₀Al₅₀ and Mn₅₄Al₄₆ alloys.

Mn-Al system Mn and Al atoms are situated in alternating planes spaced at a distance of c/2 [1].		Mn		AI		М		Total		
			<i>m</i> _s (μ _B)	<i>m</i> լ(μ _B)	<i>m</i> _s (μ _B)	<i>m</i> լ(μ _B)	<i>m</i> _s (μ _B)	<i>m</i> _l (μ _B)	<i>m</i> _s (μ _B)	<i>m</i> լ(μ _B)
Min atoms situated in <i>adjacent planes</i> (Min ^{ra} -Min ^{2e} pairs) AFM coupling .	Mn ₅₀ Al ₅₀		2.41	0.04	-0.08	-	_	-	4.68	0.08
In order to decrease the weight of the AFM interactions \implies Ni or Ti substitutions for Mn in Mn ₅₄ Al ₄₆ .	Mn ₅₄ Al ₄₆ (FM)	Mn ^{2e}	2.43	0.007	-0.08	-	-	_	5.02	0.07
Smaller Ni or Ti moments \longrightarrow increase of the total magnetic moment for $Mn_{50}AI_{46}M_4$ ($M = Ni, Ti$). Mn ₅₄ AI ₄₆ (FW)		Mn ^{1a}	2.39	0.04						
		Mn ^{2e}	-3.17	-0.01	-0.07	_	-	_	4.38	0.08
	WIN ₅₄ AI ₄₆ (AFW)	Mn ^{1a}	2.35	0.04						
Smaller total energy for a mixed 1 a and 2 e Ni occupancy than for an exclusive 2 e Ni occupancy.	Mn ₅₀ Al ₄₆ Ti ₄ Mn ₅₀ Al ₄₆ Ni ₄		2.34	0.04	-0.08	-	-0.66	-0.004	4.43	0.07
A lower total energy was found for the alloy with the AFM coupled Mn ^{1a} -Mn ^{2e} pair.			2.45	0.04	-0.08	-	0.63	0.06	4.85	0.08

Experimental Results:



[1] J. H. Park, Y. K. Hong, S. Bae, J. J. Lee, J. Jalli, G. S. Abo, N. Neveu, S. G. Kim, C. J. Choi, J. G. Lee, *J. Appl. Phys.*, **107**, 09A731 (2010).
[2] T. E. Prost, "PhD Thesis: Magnetic Properties Study of the Mn-Al System with Additions of B or C and Mechanical Milling Techniques", University of Nebraska – Lincoln, 2012.

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