Magnetism and magnetocrystalline anisotropies of ordered $L1_0$ MnPt alloy: A first principles study on bulk and thin films

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The antiferromagnetic MnPt is widely used as a pinning layer in GMR and TMR devices [1-2]. In this paper, magnetism and magnetocrystalline anisotropy (MCA) of ordered binary $L1_0$ type MnPt are studied by using density functional theory (DFT) in generalized gradient approximation (GGA). Four different spin alignments have been considered FM, A-AFM, C-AFM and G-AFM shown in Figure 1. For MnPt, the most stable phase is the C-type AFM phase with axial ratio of c/a = 0.894 which is in good agreement with the experimental results [3-4]. In this configuration, our calculations show magnetic moment of 3.745 μ_B on Mn atom and 0.096 μ_B on Pt atom along with in-plane MCA energy of 0.22 meV/atom. High temperature magnetic phase of A-type AFM is calculated to have 0.455 eV higher energy than the C-type AFM, but it is calculated to be energetically favorable compared to the FM phase. Lattice parameters, magnetic moments and MCA energies of all the magnetic configurations are catalogued in Table 1. Another silent feature observed in the DOS curve is an extremely deep TDOS minimum or pseudogap near the Fermi energy which is very sharp in C-type AFM, as shown in Figure 2. MCAs of Mn-terminated and Pt-terminated thin films are also investigated. And we will discuss strain effect on the pseudogap in TDOS.

Table 1. Lattice parameters, magnetic moments on Mn and Pt atom, total energies and MCA energies of FM, A-AFM, C-AFM, and G-AFM configurations in bulk.

	a (Å)	c (Å)	c/a	μ_{Mn}	μ_{pt}	Energy (eV)	$E^{(100-001)}$ (meV/atom)
A-AFM	4.12	3.576	0.868	3.805	0.001	0.455	0.1718
C-AFM	4.09	3.658	0.894	3.745	0.096	0.000	0.2226
G-AFM	4.10	3.614	0.880	3.708	0.000	0.633	0.3007
FM	4.14	3.537	0.855	3.830	0.394	0.651	1.240
EXP	4.00*	3.670*	0.920*	4.0±0.4*	0.4±0.4*	-----	--------

*Ref. [4]

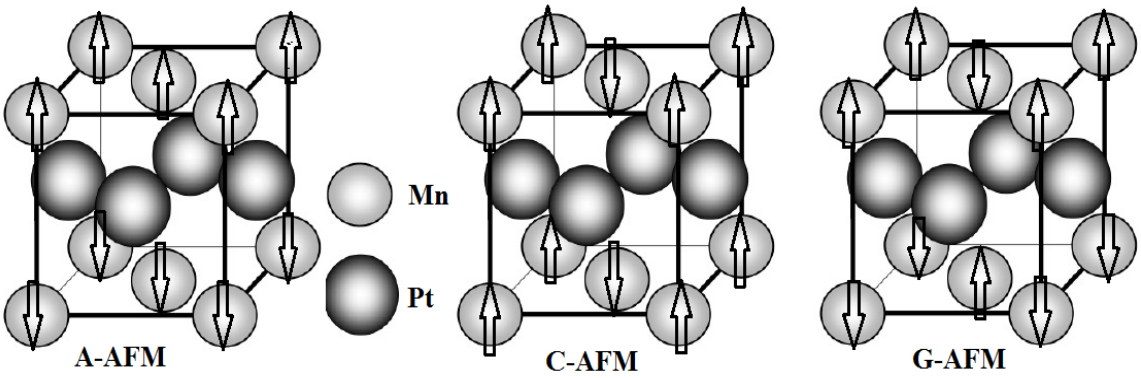

Fig. 1. Schematic diagram of A-AFM, C-AFM and G-AFM phases of $L1_0$ crystal structure.

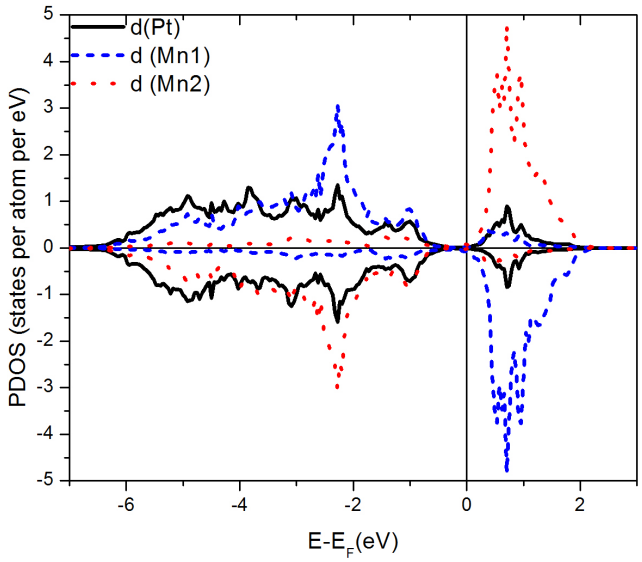

Fig. 2. d-orbital projected DOS of the C-AFM state.

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