Magnetism and magnetocrytalline anisotropies of ordered $L1_0$ MnPt alloy: A first principles study

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Spintronics of antiferromagnets is a new and rapidly developing field of the physics of magnetism [1-3]. Even without macroscopic magnetization, antiferromagnets, similar to ferromagnetic (FM) materials, are affected by spin-polarized current, and as in ferromagnets this phenomenon is based on a spin-dependent interaction between localized and free electrons. We studied electronic structure and magnetism of an ordered binary $L1_0$ type MnPt alloy by using density functional theory (DFT) in generalized gradient approximation (GGA). Four different magnetic configurations shown in Fig. 1 have been taken into account. For bulk MnPt we find Type-2 antiferromagnetic (AFM) ground state whose magnetic configuration is FM alignment in the inter-plane but AFM in the intra-plane, with c/a = 0.894 which is in good agreement with experimental results [4-5]. In this configuration, our calculations show magnetic moment of 3.745 μB on Mn atom and 0.096 μB on Pt atom and in-plane magnetocrystalline anisotropy (MCA) energy of 0.22 meV/atom. For all the magnetic configurations, lattice parameters, magnetic moments, and MCA energies are catalogued in Table 1. In addition, MCA and magnetism of Mn-terminated and Pt-terminated thin films will also be discussed.

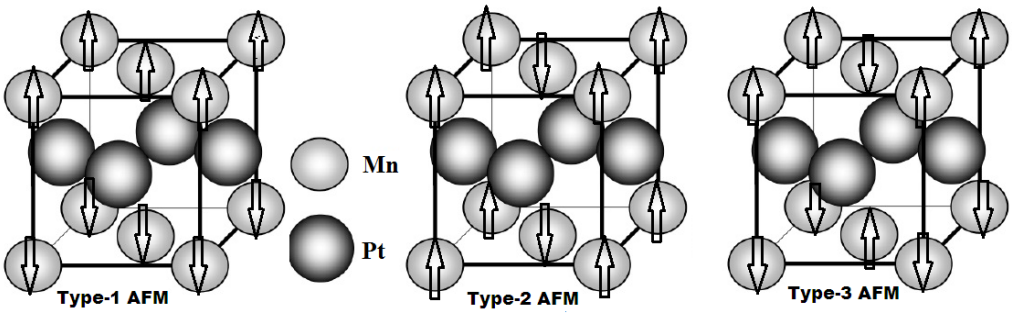

Fig. 1. Schematic diagram of Type-1 AFM, Type-2 AFM and Type-3 AFM phase for $L1_0$ crystal structure

Table 1. Calculated equilibrium lattice parameters, a (Å) and c/a, magnetic moments (in μ_B) on Mn and Pt atom, total energy difference (in eV/atom) with respect to Type-2AFM structure and MCA energies (in meV/atom) of FM, Type-1, Type-2 and Type-3 AFM configuration in bulk. Previous Theoretical results are also given for comparison.

	Type-1 AFM		Type-2 AFM		Type-3 AFM	FM	
	Present	Previous[a]	Present	Previous[a]	Present	Present	Previous[a]
a	4.12	4.10	4.09	3.99	4.10	4.14	4.17
c/a	0.87	0.87	0.89	0.93	0.88	0.86	0.84
μ_{Mn}	3.81	3.89	3.75	3.80	3.71	3.83	3.94
μ_{Pt}	0.00	0.00	0.09	0.00	0.00	0.39	0.39
ΔE	0.46		0.00		0.63	0.65	
$E^{(100\text{-}001)}$	0.17		0.22		0.30	1.24	

[a]Zhihong et al. [6]

References

[1] A. H. Macdonald Phil. Trans. R. Soc. A 369, 3098–3114 (2011).

[2] A. B. Shick, S. Khmelevskyi, O. N. Mryasov, J. Wunderlich, and T. Jungwirth Phys. Rev. B 81, 212409 (2010).

[3] Xavier Martí, IEEE transactions on magnetics, 51, 4 (2015).

[4] E. Krén, C. Kádár, L. Pál, J. Sólyom, P. Szabó, and T. Tarnóczi, Phys. Rev. 171, 574 (1968).

[5] C. S. Severin, C. W. Chen, and C. Stassis, J. Appl. Phys. 50, 4259 (1979).

[6] Zhihong Lu, Roman V. Chepulskii and W. H. Butler Phys. Rev. B 81, 094437 (2010).