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**LETTER TO THE EDITOR**

# A study of the electronic structure of $Pt_3Mn$ alloys by the LMTO method

A Jezierski†
Physics Department, Loughborough University of Technology, Loughborough, Leicestershire LE11 3TU, UK

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**Abstract.** The electronic density of states of paramagnetic and ferromagnetic ordered $Pt_3Mn$ alloys is calculated using the linear muffin tin orbital method (LMTO) and the atomic sphere approximation (ASA). The Fermi level in the ferromagnetic system is located at the dip valley between two peaks. The magnetic moments on Mn and Pt atoms are $3.64\mu_B$ and $0.22\mu_B$ respectively. These values are close to the experimental ones. The calculated value of the $\gamma$-coefficient is similar to the observed value.

Electronic and magnetic properties of Mn–Pt alloys have been studied experimentally and theoretically [1–8]. Recently, Tohyama *et al* [9] calculated the electronic density of states of a $Pt_3Mn$ alloy using the tight-binding approximation. The value of the density of states at the Fermi energy $n(E_F)$ and that of the $\gamma$-coefficient were smaller than the experimental results ($\gamma = 3.5$ mJ K$^{-2}$ mol$^{-1}$) [4], $n(E_F) = 68.1$ states Ryd$^{-1}$/cell [10]. Self-consistent spin polarised APW calculations were made by Hasegawa [11]. He found that the magnetic moment on the Mn atom was $3.8\mu_B$, but the density of states at the Fermi energy $n(E_F)$ was less than the experimental result. ($n(E_F) = 56$ states Ryd$^{-1}$/cell). He concluded that the Pt d states contribute dominantly to the density of states, while the contribution of the Mn d states is small—less than 10% of the total density of states.

In this Letter we present self-consistent spin polarised LMTO–ASA [12–13] band calculations for the ferromagnetic ordered $Pt_3Mn$ alloy.

In the ordered $Cu_3Au$- ($L1_2$-) type structure, Pt atoms are located in the centres of the faces of the cell and Mn atoms occupy the corner sites. We carried out band calculations for the paramagnetic and ferromagnetic $Pt_3Mn$ system. In an ASA the Wigner–Seitz cell is replaced by a sphere with radius $S$. The value of $S$ is determined from the condition $4\pi S^3 n/3 = V$, where $V$ is the volume of the cell and $n$ denotes the number of atoms in the primitive cell. In the band calculations we include s, p and d states of Mn and Pt. As the initial atomic configuration, we assume for Mn $3d^5$, $4s^2$, and for Pt $5d^8$, $6s^2$. The self-consistent convergence was to the value 0.001 Ryd. The band calculations were performed using the von Barth–Hedin [14] parametrisation for the local exchange correlations. The electronic density of states (DOS) was determined using

† Permanent address: Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 19, 60–179 Poznan, Poland.

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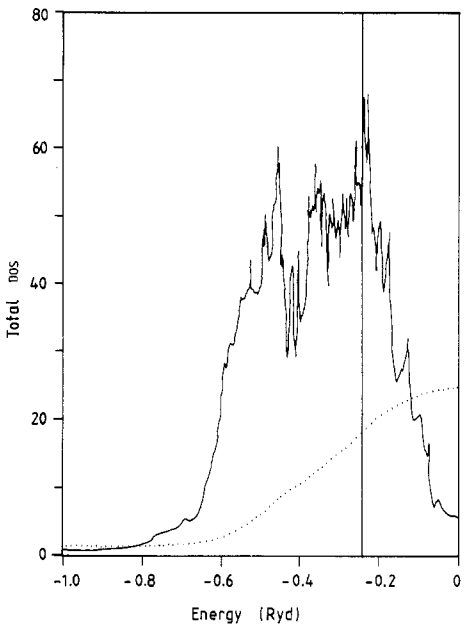


**Figure 1.** The total density of states and the total number of states (. . . . .) for paramagnetic $MnPt_3$.

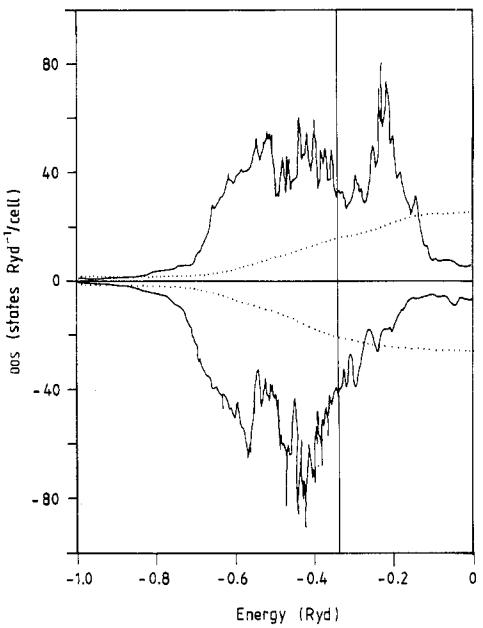


**Figure 2.** The total density of states for two directions of spin in ferromagnetic $MnPt_3$. The total number of states is also given (. . . . .) for each direction of spin.

the tetrahedron method for 85 $k$-points in the irreducible Brillouin zone. The value of $S$ is determined from the minimum of the total energy, and we obtain for the ferromagnetic system $S = 2.9$ au ($a = 3.93$ Å) which is about 1% greater than the experimental value ($a_{exp} = 3.89$ Å) [2]. LMTO corrections to the ASA method were included in the calculations.

In figure 1 we present the total density of states for paramagnetic $Pt_3Mn$ alloy. The Fermi level is located in the peak at $E_F = -0.244$ Ryd; and $n(E_F) = 74.32$ states $Ryd^{-1}$/cell. In the paramagnetic states the contributions to the total density of states at $E_F$ from Mn and Pt are almost the same.

The more interesting system is the ferromagnetic alloy. In figure 2 we have plotted the total DOS for majority spin (upper curve) and for minority spin (lower curve, denoted by negative values in the figure). The Fermi level $E_F = -0.348$ Ryd is situated in the dip valley between two subpeaks. The large peak on the right hand side of $E_F$ gives the contribution from Mn. The total density of states at the Fermi energy is larger than in the previous calculations [9, 11]. We obtain $n(E_F) = 72.34$ states $Ryd^{-1}$/cell for the ferromagnetic $Pt_3Mn$ alloy. The dotted curve in figure 2 represents the total number of states. In table 1 we list the partial and total densities of states at $E_F$. The contribution from the Mn to the total $n(E_F)$ is about 14% and the main contribution is due to Pt. In the last three columns in table 1 we present the previous theoretical calculations [9, 11] and the experimental values of the total density of states at $E_F$ [10]. Using the total value of $n(E_F)$ we estimated the $\gamma$-coefficient in $Pt_3Mn$. We obtained $\gamma = 3.13(1 + \lambda)$ which is close to the experimental value ($\gamma = 3.5$ mJ $K^{-2}$ $mol^{-1}$ [4]). Our self-consistent spin polarised band calculations indicate that the value of $\lambda$ should be small ($\lambda \simeq 0.12$).

**Table 1.** Density of states at $E_F$ (states $Ryd^{-1}$/cell) in ferromagnetic $Pt_3Mn$.

| | | | | | Theory | | Experiment |
|---|---|---|---|---|---|---|---|
| | s | p | d | Total | [9] | [11] | [10] |
| $Pt_3Mn$ | 4.73 | 6.52 | 61.09 | 72.34 | 40 | d 56.0 | 68.1 |
| Mn | 1.22 | 1.48 | 16.13 | 18.83 | | d 5.0 | |
| 3Pt | 3.51 | 5.04 | 44.96 | 53.51 | | d 44.0 | |

**Table 2.** Local and total magnetic moment in $Pt_3Mn$ (in $\mu_B$).

| | | | | | Theory | | Experiment |
|---|---|---|---|---|---|---|---|
| | s | p | d | Total | [9] | [11] | [1, 3] |
| Mn | 0.06 | 0.05 | 3.53 | 3.64 | 4.24 | 3.8 | $3.64 \pm 0.08$ |
| Pt | 0.003 | 0.04 | 0.18 | 0.22 | 0.14 | 0.2 | $0.26 \pm 0.03$ |
| Total ($Pt_3Mn$) | 0.07 | 0.16 | 4.08 | 4.30 | | 4.2 | 3.9[1], 4.4[3] |

In table 2 we list the local and total magnetic moment. The values of the magnetic moment of Mn and Pt atoms are in good agreement with experimental data [1, 3].

We obtained for the Mn d electrons the LSD Stoner parameter $U = 0.059$ Ryd, which is close to the Andersen *et al* [13] and Janak [15] values. Band splittings were obtained from the self-consistent potential parameters, following Andersen [12]. The splitting of the d bands of Mn is $\Delta = 0.209$ Ryd; however, for Pt d bands it is $\Delta = 0.01$ Ryd. Our results confirm the general shape of the density of states in $Pt_3Mn$ ordered alloy, and our values of the magnetic moments and $\gamma$-coefficient are very close to experimentally measured values.

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