# First-principles studies of magnetic properties of CoFePd multilayers

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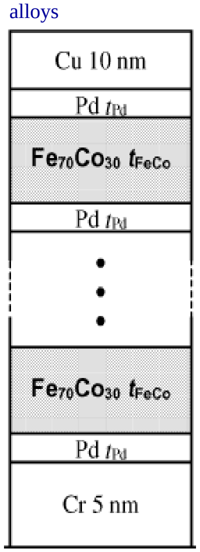
### Abstract

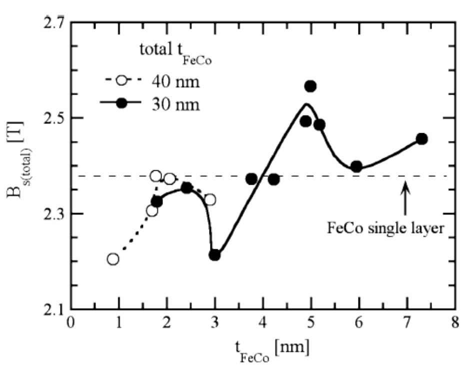
Enhancement of the saturation magnetization above that achievable in the bcc FeCo alloy system is greatly desired for use in the write pole in magnetic recording. Recent reports by Noma et al.[1] as well as earlier reports indicate that adding small amounts of Pd to high magnetization FeCo alloys or interspersal of thin layers of Pd in these alloys may enhance their magnetization. In order to investigate this possibility, we have performed ab-initio studies of FeCoPd alloys and of multilayers of FeCo and Pd. Supercells representing 3 atomic layers of $Fe_{75}Co_{25}$ alternating with 1 atomic layer of Pd in (100) or (110) directions consisted of 16 atoms, i.e. 4 Pd, 9 Fe and 3 Co (4 atoms per layer). Both structures were structurally relaxed in shape and volume. The magnetic moments and magnetizations of these supercells were compared to those of supercells consisting entirely of 4 layers of $Fe_{75}Co_{25}$ (12 Fe and 4 Co atoms). We have also investigated much larger cells consisting of 24 atomic layers in the (110) direction. These cells were designed to model the results of ref.[1].


[1] K. Noma, M. Matsuoka, H. Kanai, Y. Uehara, K. Nomura, N. Awaji, IEEE TRANSACTIONS ON MAGNETICS, 41 (2005) 2920, *ibid.* 42 (2006) 140).

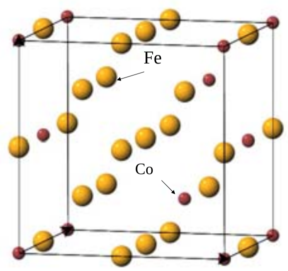
▪ Below is show results of an experiment by Noma et al. [1] in which they reported up to 2.57 T saturation magnetization in $Co_{30}Fe_{70}Pd$ multilayers and alloys



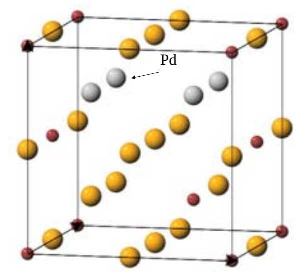

K. Noma et al., IEEE TRANSACTIONS ON MAGNETICS, 41 (2005) 2920; *ibid.* 42 (2006) 140

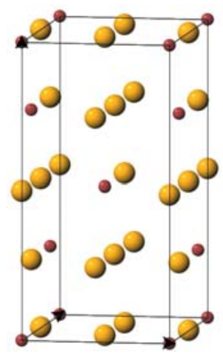



• Calculations are based on density functional theory (DFT) with generalized gradient approximation (GGA) for exchange correlation potential using VASP
• Full structural relaxation in shape and volume was performed.



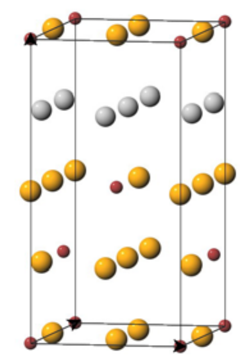

| 100 cells | $Co_{25}Fe_{75}$ | $Co_{25}Fe_{75}Pd$ | $Co_{25}Fe_{75}$ sublattice |
|---|---|---|---|
| Volume (Å$^3$) | 184.94 | 206.17 | 143.12 |
| Magnetic moment ($\mu_B$) | 37.42 | 31.27 | 31.27 |
| Magnetization ($10^6$ A/m) | 1.876 | 1.406 | 2.026 |
| Flux density (T) | 2.358 | 1.767 | 2.546 |



16 atom (100) and (110) cells with 4 atoms per layer:
• Left panels shows $Co_{25}Fe_{75}$ with 1 Co, 3 Fe per layer
• Right panels shows Co25Fe75 with 1 Co, 3 Fe per layer

| 110 cells | $Co_{25}Fe_{75}$ | $Co_{25}Fe_{75}Pd$ | $Co_{25}Fe_{75}$ sublattice |
|---|---|---|---|
| Volume (Å$^3$) | 184.93 | 205.6 | 148.73 |
| Magnetic moment ($\mu_B$) | 37.06 | 30.59 | 30.59 |
| Magnetization ($10^6$ A/m) | 1.859 | 1.38 | 1.907 |
| Flux density (T) | 2.335 | 1.734 | 2.397 |



To model 5 nm thick multilayers we performed calculations on 48 and 96 atom (110) cells with 4 atoms per layer

| 110 cells | 48 atoms cell (24 layers) | | | 96 atoms cell (24 layers) | | |
|---|---|---|---|---|---|---|
| | $Co_{30}Fe_{70}$ | $Co_{30}Fe_{70}Pd$ | $Co_{30}Fe_{70}$ sublattice | $Co_{30}Fe_{70}$ | $Co_{30}Fe_{70}Pd$ | $Co_{30}Fe_{70}$ sublattice |
| Volume (Å$^3$) | 553.86 | 567.86 | 536.7 | 1104.39 | 1124.76 | 1064.39 |
| Magnetic moment ($\mu_B$) | 110.87 | 108.42 | 108.42 | 222.14 | 214.51 | 214.51 |
| Magnetization ($10^6$ A/m) | 1.85 | 1.77 | 1.87 | 1.865 | 1.769 | 1.869 |
| Flux density (T) | 2.33 | 2.23 | 2.35 | 2.344 | 2.222 | 2.349 |

**Conclusion:**

• In all results above we consistently find that addition of Pd may raise the FeCo sublattice magnetization, but that the total magnetization is decreased.