Magnetism in Pd Particles

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Careful first-principles calculations [1] indicate that, contrary to the face centered cubic phase which is paramagnetic, the hexagonal close-packed phase of Pd is ferromagnetic with a magnetic moment of the order of 0.35 μ_B per atom. Moreover, our results show that the presence of two dimensional defects with local hcp stacking of layers like twin boundaries and stacking faults in the otherwise fcc Pd structure, induces non vanishing local magnetic moments arranged in ferromagnetic order. These results are consistent wit experiments in small Pd clusters [2] where small Pd particles of average diameter 2.4 nm are reported to display spontaneous magnetization. High-resolution transmission electron microscopy (see the below Figure) have shown that a high percentage of the fcc particles exhibit single and multiple twinning boundaries. In addition, the smallness of the spontaneous magnetization seems to indicate that only a small fraction of atoms holds a permanent magnetic moment and contributes to ferromagnetism.

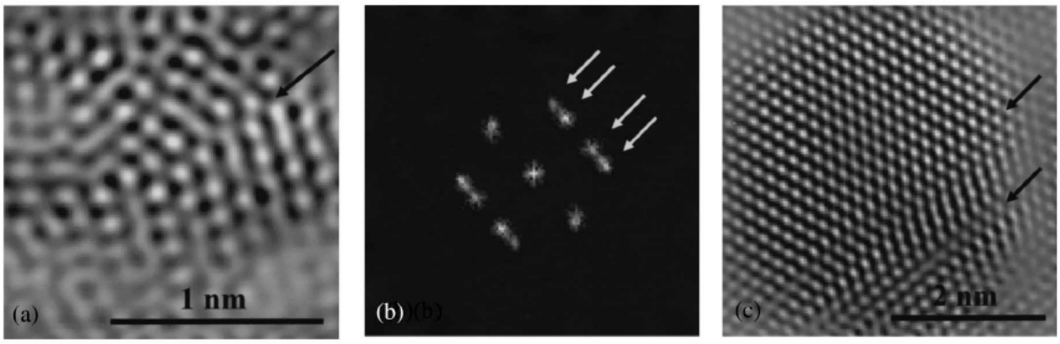

Figure 1. High resolution transmission electron microscopy images of Pd particles (ref. [2]).

The main conclusions of our work [1] can be summarized as follows:

(a) Pd in the hcp phase is in the ferromagnetic side, close to a magnetic non-magnetic transition. The fcc paramagnetic phase being lower in energy by 38 meV.
(b) Stacking-faults and twin boundaries, when clustered, are magnetic. Our calculations have gone up to stacking-faults separated by twelve fcc layers. Beyond these separations between the faults the calculations become unreliable since we have not obtained results satisfying the stringent convergency criteria used in this work. Therefore, for the time being, we cannot assess whether or not isolated faults are magnetic. The Figure below shows the magnetic moment when the stacking faults, with the local hp structure, are separated by six fcc layers. Similar results are obtained for separations up to twelve fcc layers.

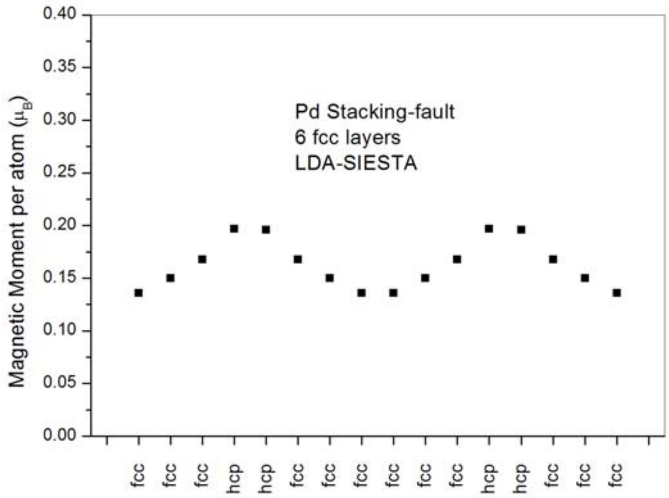

Figure 2. Magnetic moment at the atoms around stacking-faults separated by six fcc layers [1].

(c) Recent experimental results [3] on small Pd particles, different from those of ref. [2], have also shown their ferromagnetic character. The interpretation in this case is that the (100) facets of the clusters are responsible for the appearance of magnetism in the particles. Based on our calculations in different size slabs, we can rule out the experimental interpretation in terms of surface and/or atomic relaxation induced magnetism.

(d) Magnetic anomalies observed experimentally in different Ni [4] and Co [5] stackings in nanoparticles deposited on top of Cu can be interpreted along the lines described in this work.

We have shown that, in palladium, deviations from the ideal fcc crystal structure like stacking-faults and twin boundaries, present in nanoparticles, can induce the magnetization of the atoms at the defect and its fcc surroundings. The high magnetic susceptibility of the stable fcc structure close to a non-magnetic/magnetic transition is responsible for this effect that can also take place in other non ideal structures like nanowires [6].

References

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