STRENGTH AND MAGNETISM OF NANOCOMPOSITES FORMED BY 3D-METAL NANOCHAINS EMBEDDED IN A NON-MAGNETIC MATRIX

M. Šob[1,2,3] and T. Káňa[3]

[1]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic
[3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

Introduction

The recent findings of structure transitions in Fe, Ni [1] and Mn [2] nanowires stimulated our interest in ab initio simulation of tensile tests of nanocomposite metallic materials. Among others, our aim was to study Mn−Pt compounds and nanocomposites, in particular the recently found ordered $MnPt_7$ structure, and find the relation between its mechanical and magnetic properties. Another interesting topic is the $MnPt_{15}$ compound, which represents a natural nanocomposite with Mn or Mn−Pt nanochains oriented along the [100], [110] and [111] directions. It turns out that some of these configurations are stabilized by antiferromagnetic ordering and magnetic moments of manganese atoms may be coupled through the platinum atoms.

Computational details

For the ab initio total-energy calculations, we employed the full-potential linearized augmented-plane wave (FLAPW) method implemented in the WIEN2k code [3]. Exchange-correlation energy was determined within the local density approximation (LDA) [4]. The spin-orbit coupling was not included and our calculations were restricted to collinear magnetism. The values of calculated magnetic moments at individual atoms correspond to electrons inside the muffin-tin spheres.

Results and discussions

First, we have calculated the elastic constants c_{11}, c_{12} and c_{44} of elemental Pt and performed ab initio tensile tests along the ⟨100⟩ and ⟨111⟩ directions. Our values of maximum tensile stress $\sigma_{max,0}$ and the corresponding strain $\varepsilon_{max,0}$ were in a good agreement with previous results [5, 6]. The same calculations were carried out for the ferromagnetic compound $MnPt_3$ and for the novel compound $MnPt_7$. For $MnPt_7$, we have found the antiferromagnetic ground-state (see Fig. 1), similarly as it was revealed experimentally for the Pt−8.8 at. % Mn alloy [7].

The effect of manganese doping on platinum matrix consists in its softening − the bulk modulus B and elastic constants c_{11} and c_{12} are reduced. On the other hand, the Mn-doped structures are more resistant against shape deformation and exhibit an increase in the Young moduli E_{100}, E_{111} and shear moduli c_{44} and

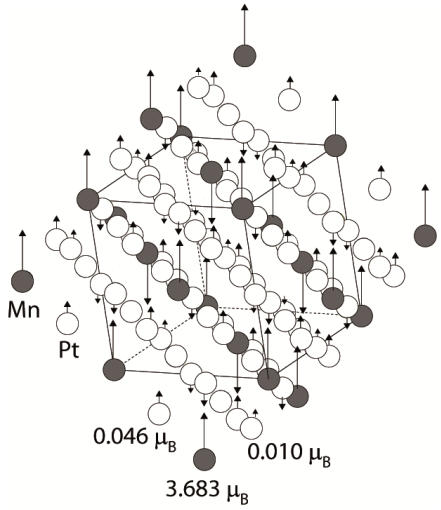

Fig. 1. The antiferromagnetic (AFM [100]) ordering of the $MnPt_7$ structure corresponds to its ground state.

(c_{11} - c_{12})/2. The maximum tensile stress $\sigma_{max,0}$ and the maximum corresponding strain $\varepsilon_{max,0}$ are not affected too much by Mn doping, exhibiting only a slight increase. In comparison with elemental Pt, the maximum tensile stress of the compound $MnPt_3$ in the directions ⟨100⟩ and ⟨111⟩ increases by 4.2 % (to 37.0 GPa) and by 6.7 % (to 33.3 GPa), respectively. On the other hand, the corresponding maximum strain $\varepsilon_{max,0}$ of $MnPt_3$ decreases by 8.4 % to 0.305 and by 9.0 % to 0.218, respectively. The values of the maximum tensile stress of $MnPt_7$ in the antiferromagnetic ground state are very close to those of elemental Pt; they amount to 35.6 GPa for the loading along the ⟨100⟩ direction and 30.6 GPa for the loading along the ⟨111⟩ direction. The latter value is even by 2.1 % lower than that of elemental Pt. The values of maximum corresponding strain in $MnPt_7$ are 0.317 and 0.232. They lie between the values for $MnPt_3$ and elemental Pt.

Further, we have also investigated the preferential occupation of Mn atoms in the Pt matrix and confirm the experimental result that they prefer the positions at the corners and at the centers of faces of the 2x2x2 Pt supercell. Our modeled structures denoted as $MnPt_{15}$ have 6.25 at. % of manganese and can be regarded as natural linear nanocomposites. They may be considered as an assembly of Mn or Mn−Pt nanochains embedded in Pt matrix. These nanochains can be oriented along the [100], [110] or [111]

directions. We found that the "base-centered" structure with the stripped Mn-Pt nanochains along the [110] direction has the lowest energy among these structures and is stabilized by antiferromagnetic ordering (see Fig. 2). However, an alternative ferromagnetic ordering (Fig. 3) has the total energy only by 3.3 meV/atom higher. Moreover, the calculated screening of spins of Mn atoms by flipping the spins of some Pt atoms indicates that the spins of Mn atoms can be coupled through the Pt atoms, similarly as spins of atoms in Mn dimers on CuN substrate are coupled by nitrogen atoms [8].

The total energy of the atomic configuration with nanochains along the [100] direction (not shown) is by 4.6 meV/atom higher than that of the antiferromagnetic "base-centered" configuration. The ferromagnetic and antiferromagnetic orderings of this configuration are nearly degenerate. On the other hand, the configuration with Mn nanochains oriented along the [111] direction favors ferromagnetism by 0.2 meV/atom. We observe a decrease of magnitudes of magnetic moments induced on Pt atoms when the structures are ordered antiferromagnetically.

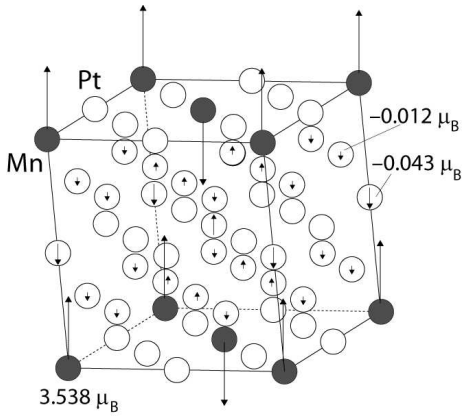

Fig. 2. The antiferromagnetic ordering of the $MnPt_{15}$ structure in the configuration "base-centered". The Mn−Pt nanochains embedded in the Pt matrix are oriented along the [110] direction.

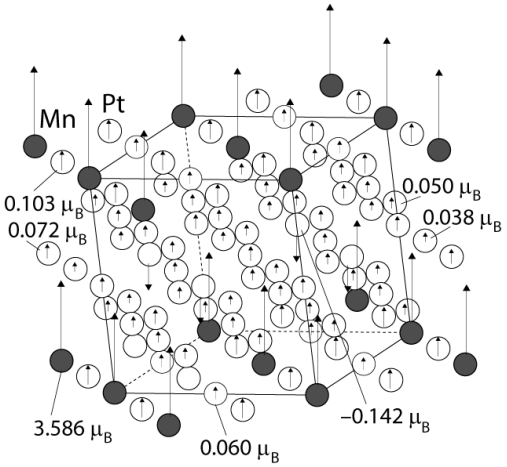

Fig. 3. An alternative ferromagnetic ordering of the $MnPt_{15}$ structure in the configuration "base-centered". The Pt atoms at the centers of the faces of the 2x2x2 supercell screen the magnetic moments of Mn atoms.

Conclusions

In summary, we have studied the effect of Mn doping in platinum and found an increase of shear moduli $(c_{11} - c_{11})/2$ and c_{44} and little increase of maximum tensile stress $\sigma_{max,0}$. On the other hand, the manganese dopants act as softening agent to Pt matrix, reducing the lattice constant *a*, bulk modulus *B* and the values of elastic constants c_{11} and c_{12}. The maximum strain $\varepsilon_{max,0}$ corresponding to the maximum tensile stress is slightly reduced, too.

We have modeled several Mn−Pt compounds and nanocomposites, in particular the recently found $MnPt_7$ (super)structure, and determined the antiferromagnetic ordering as its ground state. A similar antiferromagnetic ordering has been found in our model $MnPt_{15}$ structure. The last result is in agreement with experiment, for this antiferromagnetic ordering has been found experimentally in the Pt−8.8 % Mn alloy with manganese concentration similar to $MnPt_{15}$. We studied also magnetic states of linear nanocomposites consisting of Mn or Mn−Pt nanochains in the Pt matrix. Our results indicate the existence of a coupling of Mn spins through the surrounding Pt atoms.

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