

MECHANICAL AND MAGNETIC PROPERTIES OF Mn-Pt COMPOUNDS AND NANOCOMPOSITES

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Abstract

An analysis of mechanical and magnetic properties of Mn-Pt compounds and nanocomposites is provided using DFT calculations. Adding manganese to platinum matrix reduces the bulk modulus and enhances the Young moduli and shear moduli. With increasing Mn content, the theoretical tensile strength is also enhanced and the corresponding maximum deformation is reduced. On the whole, manganese addition makes the Mn-Pt compounds softer, but increases their resistance to shape deformation. Many of these compounds may be considered as natural linear nanocomposites. We studied the magnetic configurations of recently found MnPt₇ ordered structure and predict an antiferromagnetic state with spins altering along the [100] direction to be the ground state of this compound. The ferromagnetic state and an alternative antiferromagnetic state with spins altering along the [111] direction have a higher total energy. We further studied Mn-Pt nanocomposites exhibiting the composition of MnPt₁₅. The preferential occupation of Mn atoms are the corners and centers of the faces of the 2x2x2 supercell. Such a structure with an antiferromagnetic ordering with spins altering along the [100] direction is the ground state of MnPt₁₅ nanocomposite. Contrary to MnPt₇, the alternative ferromagnetic configurations of different MnPt₁₅ nanocomposites exhibit the screening of magnetic moments of Mn atoms by flipping the moments induced on Pt atoms in the opposite direction. This indicates that the Mn spins can be coupled through the Pt atoms similarly as spins of Mn dimers on CuN substrate can be coupled through nitrogen atoms.

1 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 MnPt₇ structure, and find the relation between its mechanical and magnetic properties. Another interesting topic is the MnPt₁₅ 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.

2 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.

3. Results and Discussion

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 MnPt₃ and for the novel compound MnPt₇. For MnPt₇, 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 $(c_{11} - c_{12})/2$. The maximum tensile stress $\sigma_{\max,0}$ and

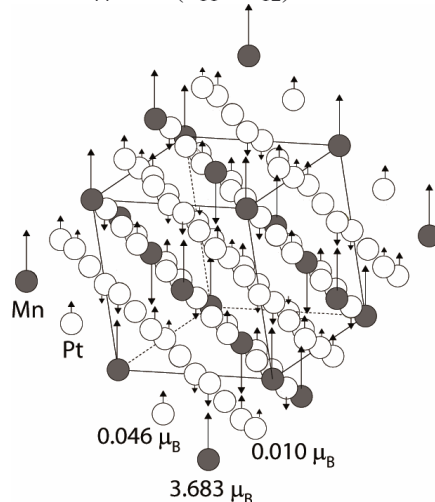


Fig. 1. The antiferromagnetic (AFM [100]) ordering of the MnPt₇ structure corresponds to its ground state.

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 MnPt₃ 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 MnPt₃ decreases by 8.4 % to 0.305 and by 9.0 % to 0.218, respectively. The values of the maximum tensile stress of MnPt₇ 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 MnPt₇ are 0.317 and 0.232. They lie between the values for MnPt₃ 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 MnPt₁₅ 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.

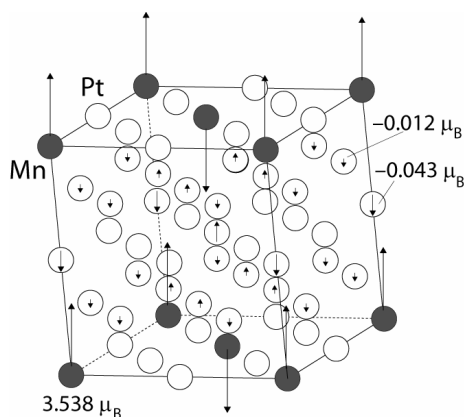


Fig. 2. The antiferromagnetic ordering of the MnPt_{15} structure in the configuration "base-centered". The Mn–Pt nanochains embedded in the Pt matrix are oriented along the [110] direction.

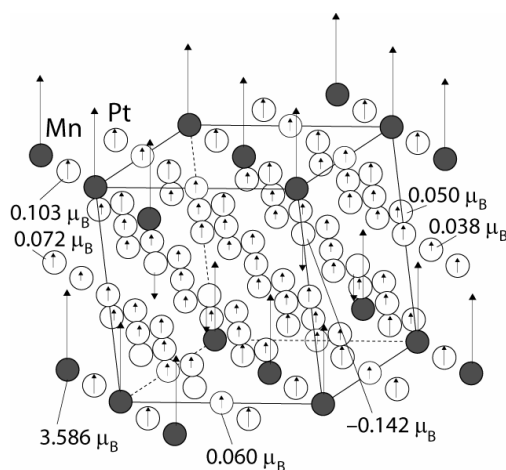


Fig. 3. An alternative ferromagnetic ordering of the MnPt_{15} structure in the configuration "base-centered". The Pt atoms at the centers of the faces of the $2 \times 2 \times 2$ supercell screen the magnetic moments of Mn atoms.

4 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 MnPt₇ (super)structure, and determined the antiferromagnetic ordering as its ground state. A similar antiferromagnetic ordering has been found in our model MnPt₁₅ 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 MnPt₁₅. 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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