MECHANICAL AND MAGNETIC PROPERTIES OF MN-PT COMPOUNDS AND NANOCOMPOSITES

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Abstract

Using ab initio calculations, we have analysed behaviour of Mn atoms dissolved in a platinum matrix, forming thus intermetallics MnPt3, MnPt7 and MnPt15 that can be considered as prototypes of natural Mn–Pt nanocomposites. On the whole, manganese addition makes the resulting Mn–Pt compound softer, but increases its resistance to shape deformation. In particular, dissolved Mn atoms form a superstructure with the platinum matrix with reduced bulk modulus and enhanced Young moduli E100, E111 and shear moduli (c11 - c12)/2 and c44. With increasing Mn content, the theoretical tensile strength is also enhanced and the corresponding maximum deformation is reduced. From the magnetic point of view, we have found a cascade of magnetic ground states: from non-magnetic Pt through the recently found antiferromagnetic MnPt7 up to the ferromagnetic MnPt3. Our systematic study shows that the resulting magnetic ordering of Mn atoms in the Pt matrix depends on their mutual distance. In agreement with experiment, our calculations confirm the antiferromagnetic (AFM) ground state of the MnPt7 structure with spins directions alternating along the [100] crystallographic direction (AFM [100]). This ground state is preferential to the speculated AFM state with spins directions alternating along the [111] crystallographic direction (AFM [111]). We show that the AFM [100] ordering preserves the cubic symmetry of the MnPt7 crystal structure whereas the AFM [111] does not. In addition, we have proposed and studied three prototypes of linear MnPt15 nanocomposites consisting of Mn nanochains in the Pt matrix.

Keywords: nanocomposites, magnetism, ab initio calculations

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