Ab initio study of mechanical and magnetic properties of Mn-Pt compounds and nanocomposites

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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 $MnPt_7$ 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 $MnPt_{15}$. The preferential occupation sites 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 $MnPt_{15}$ nanocomposite. Contrary to $MnPt_7$, the alternative ferromagnetic configurations of different $MnPt_{15}$ 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 [Phys. Rev. B 83, 014413 (2011)].

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