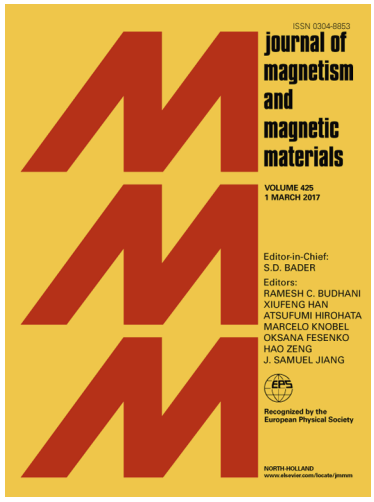

Ab initio study of the theoretical strength and magnetism of the Fe−Pd, Fe−Pt and Fe−Cu nanocomposites

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Ab initio study of the theoretical strength and magnetism of the Fe–Pd, Fe–Pt and Fe–Cu nanocomposites

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Abstract

We studied the Fe–Pd, Fe–Pt and Fe–Cu nanocomposites formed by Fe nanowires embedded in the fcc Pd, Pt or Cu matrix. The Fe atoms form nanowires oriented along the [001] crystallographic direction. They replace second nearest neighbor atoms in the matrix. By means of varying the distance between the nanowires we arrived to the chemical compositions $X_{15}Fe$, X_8Fe and X_7Fe where X stands for Pd, Pt and Cu. The mechanical and magnetic properties of the nanocomposites were obtained by ab initio simulations. We performed tensile and compressive tests along the [001] direction and compared the results with the deformation behavior of the fcc matrix and the known intermetallic compounds $FePd_3$ and $FePt_3$. It turned out that the maximum attainable stress for the Fe–Pd and Fe–Pt nanocomposites is higher than the stress attainable for the Pd and Pt matrices. The maximum stress increased with the increasing Fe content. The increase was due to the enhanced stability in the nanocomposites described by the $C_{11} - C_{12} > 0$ condition. This effect was particularly pronounced in the Fe–Pt nanocomposites. On the contrary, the Fe nanowires in the Fe–Cu nanocomposites do not enhance the stability and strength of the Cu matrix. They even make the Cu matrix more compliant to compression. Regarding the magnetic ground states, the Fe–Pd and Fe–Pt nanocomposites prefer a ferromagnetic configuration where the spins of all Fe atoms are oriented in parallel manner. On the other hand, the Fe–Cu nanocomposites exhibit an antiferromagnetic configuration where the spins of all Fe atoms assigned to a particular nanowire are oriented parallel, but antiparallel to the spins of a neighboring Fe nanowire. The Young modulus E_{001} along the [001] crystallographic direction increases linearly with the Fe content in both the Fe–Pd and Fe–Pt nanocomposites.