Thermodynamics and Kinetics-driven Dual States in FeMn(PSi) Alloys

Guijiang Li,1 Levente Vitos1,2,3

1Applied Materials Physics, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden
2Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Uppsala, Sweden
3Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest, Hungary
levente@kth.se

Fe2P-type alloys have been an interesting research topic because of the potential application as magneto-caloric materials and also because of the rich physical properties for fundamental research. We have investigated the magnetic exchange interactions, microscopic theory of magnetism, magneto-elastic effect, the magneto-structural coupling in Fe2P-type alloys as well as the phase stability of FeMnPSi alloys.

Here we report on thermodynamic-state and kinetic-process dependent dual magnetic states in FeMn(PSi) alloys. Our investigations are based in density functional theory formulated within the exact muffin-tin orbitals method in combination with the coherent potential approximation. We identify both ferromagnetic and antiferromagnetic states in FeMnP0.75Si0.25 [1] and confirm the co-existence of dual ferromagnetic orders in FeMnP0.55Si0.45 [2]. We discuss that the thermodynamic state in the high temperature paramagnetic phase and the kinetic diffusion process upon cooling co-determine the magnetic order at low temperature. The results suggest that careful control of the kinetic diffusion process in FeMnPSi alloys serves as another tuning parameter when searching for new magnetocaloric candidate materials.

Key Words: magnetocaloric, FeMnPSi, density functional, alloy theory

References