Phase Transition and Caloric Effect in MnCoGe-Based Alloys

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MnCoGe-based alloys, with a martensitic transition from orthorhombic to hexagonal,[1] are promising candidates for room-temperature magnetic refrigeration. These alloys have received considerable interest over the years because of the several advantages: (i) a strong magneto-structural coupling can be easily established and highly tuned between the Curie temperatures of two phases by elemental substitution; (ii) the featured paramagnetic-ferromagnetic-type magneto-structural transition (MST) leads to a higher entropy change than other magnetocaloric effect (MCE) materials during martensitic and magnetic transitions. However, the first-order nature of the MST inevitably results in the occurrence of thermal and magnetic hysteresis, which usually reduce the cooling efficiency. In this work,[2,3,4] we report a detailed study on the kinetic origin of hysteresis in MnCoGe-based alloys by combining *ab initio* calculations and neutron power diffraction (NPD) with magnetic and heat measurements. In an attempt to obtain the relationship between the intrinsic properties and hysteresis, the non-magnetic In atom with larger atomic radius and lower electron number are introduced to partially (2%) replace the atoms on magnetic Co or non-magnetic Ge sites, respectively. Our *ab initio* calculations reveal that MnCo($Ge_{0.98}In_{0.02}$) has a lower energy barrier compared to Mn($Co_{0.98}In_{0.02}$)Ge, leading a narrower hysteresis. Meanwhile, we have successfully synthesized these two distinct samples and a narrower hysteresis of phase transition is verified in MnCo($Ge_{0.98}In_{0.02}$). Our measurements show that the barocaloric entropy change (ΔS_P) of 20.6 J kg^{-1} K^{-1} for MnCo ($Ge_{0.98}In_{0.02}$) is slightly smaller than that of 25.1 J kg^{-1} K^{-1} for Mn($Co_{0.98}In_{0.02}$) Ge at 1 kbar, but it results in a more desirable reversible isothermal entropy change (ΔS_{rev}) of 15.9J kg^{-1} K^{-1}, which is ~1.7 times larger than that of Mn($Co_{0.98}In_{0.02}$)Ge (9.2 J kg^{-1} K^{-1}) because of the advantages of narrower hysteresis, thus making it more promising for solid-state refrigeration.

This work was supported by the National Natural Science Foundation of China (Nos. 92263202 and 12374020), the Strategic Priority Research Program of the CAS (No. XDB33000000).

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