Structural and physical properties of the *A*-site ordered perovskite manganites $RBaMn_2O_6$ (R = Pr, $Pr_{1/2}Nd_{1/2}$, and Nd)

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Introduction

Half-doped $RBaMn_2O_6$ (R – rare earth) manganites can be synthesized either in the *A*-site ordered or disordered form. These two phases exhibit different magnetic, resistive and structural properties. For example, the Curie temperature T_C of the layer ordered $LaBaMn_2O_6$ phase is 80 K higher than that of its disordered $La_{0.5}Ba_{0.5}MnO_3$ counterpart [1]. The tight correlation among the spin, charge, orbital, and lattice degrees of freedom in these manganites gives rise to complex phase competition and a rich phase diagram. Competition among antiferromagnetic (AFM), ferromagnetic (FM), and charge/orbital ordered (CO/OO) states produces dramatic changes in physical properties. For example, the colossal magnetoresistance effect arises near the AFM/FM critical point at which the application of a magnetic field rapidly induces the transition from an insulating AFM state to a metallic FM state [2].

Methods and Materials

The temperature and magnetic field dependent structural and physical properties of the half-doped *A*-site ordered manganites $RBaMn_2O_6$ (R = Pr, $Pr_{1/2}Nd_{1/2}$, and Nd) have been studied using high-resolution high-energy x-ray powder diffraction and transport and magnetic measurements. Polycrystalline materials were synthesized using a two-step solid state reaction method.

Results

The AFM to FM phase transitions of all three materials are accompanied by first-order structural changes (the results for $Pr_{1/2}Nd_{1/2}BaMn_2O_6$ presented in Fig. 1). The phase-transition temperature, T_N, increases with decreasing A-site ionic radius, and can be lowered by 15–25 K in a magnetic field of 6 T. Both phases of $PrBaMn_2O_6$ and $Pr_{1/2}Nd_{1/2}BaMn_2O_6$ have tetragonal structures (space group P4/mmm), though the ferromagnetic phase of $Pr_{1/2}Nd_{1/2}BaMn_2O_6$ shows significant broadening of the (200)/(020) diffraction peak, suggesting a slight orthorhombic distortion of the tetragonal cell. $NdBaMn_2O_6$ is tetragonal (P4/mmm) in the antiferromagnetic phase and orthorhombic (Pmmm) in the ferromagnetic phase. A giant magnetostrictive effect in this system is observed. The sudden elongation in the the basal ab-plane and the significant contraction along the c-direction of crystal structure, associated with the FM-to-AFM magnetic phase transition, indicate a strong spin-lattice coupling in this system. This transition is associated with the colossal magnetoresistance effect. The largest observed magnetoresistance is above 2000% for $NdBaMn_2O_6$ at 285 K in H = 7 T.

Discussion

The previously unobserved orthorhombic distortions in the FM phases of $NdBaMn_2O_6$ and $Pr_{1/2}Nd_{1/2}BaMn_2O_6$ suggest that orthorhombic strain is a critical parameter in the competition between FM and CO/OO in $RBaMn_2O_6$. The anisotropy reversal in the AFM/FM transition may be explained in terms of a change in the e_g electron orbital state from $d_{x^2-y^2}$ in the AFM phase to $d_{3z^2-r^2}$ in the FM phase.

Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38 and work at NIU by NSF (DMR-0302617) and the U. S. Department of Education.

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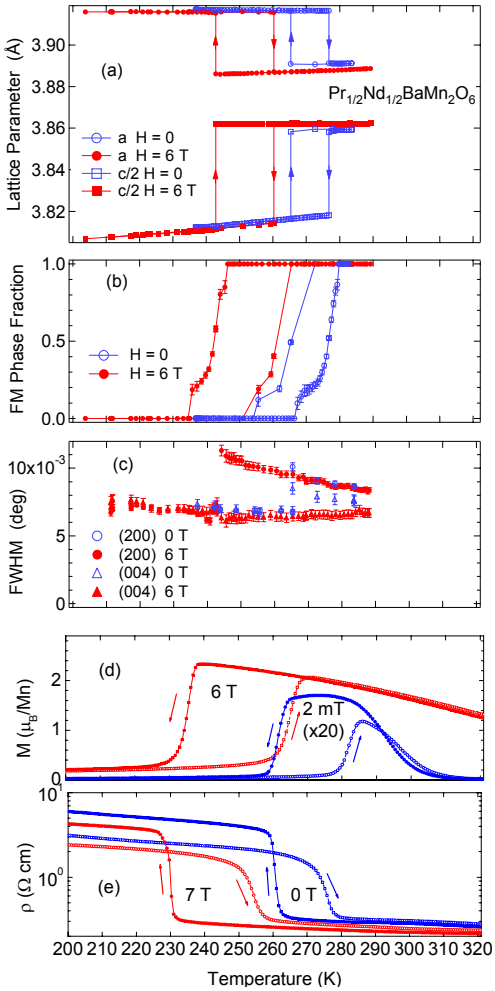

Fig. 1. Temperature- and magnetic field-dependence of structural and physical properties of $Pr_{1/2}Nd_{1/2}BaMn_2O_6$: (a) the tetragonal lattice parameters, (b) the fraction of FM phase, (c) the FHWM's of the diffraction peaks (d) magnetization, and (e) electrical resistivity.