Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Effect of cobalt doping on the structural, magnetic and abnormal thermal expansion properties of $NaZn_{13}$-type $La(Fe_{1-x}Co_x)_{11.4}Al_{1.6}$ compounds

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I. The calculated method details of the Fe^{I}–Fe^{II} distance

In order to investigate the relationship between Co content x and the Fe-Fe interatomic distance, the first-principles geometry optimization calculations for $La(Fe_{1-x}Co_x)_{11.4}Al_{1.6}$ (x = 0, 0.04, 0.06 and 0.08) are performed using the plane-wave pseudopotential method[1] implemented in CASTEP package.[2] Virtual Crystal Approximation (VCA)[3,4] is also implemented in the calculations for the statistical distribution in the periodic structure. The normal-conserving pseudopotential[5] and the generalized gradient approximation (GGA) with Perdew, Burke and Emzerhof (PBE) functionals[6] are chosen to describe the exchange and correlation (XC) potentials in the calculation of the optical properties. The plane-wave cutoff energy was set at 550eV and the Monkhorst-Pack k-point meshes[7] were set with a density of 4×4×4 points in the Brillouin zone.

II. Variable-temperature XRD patterns

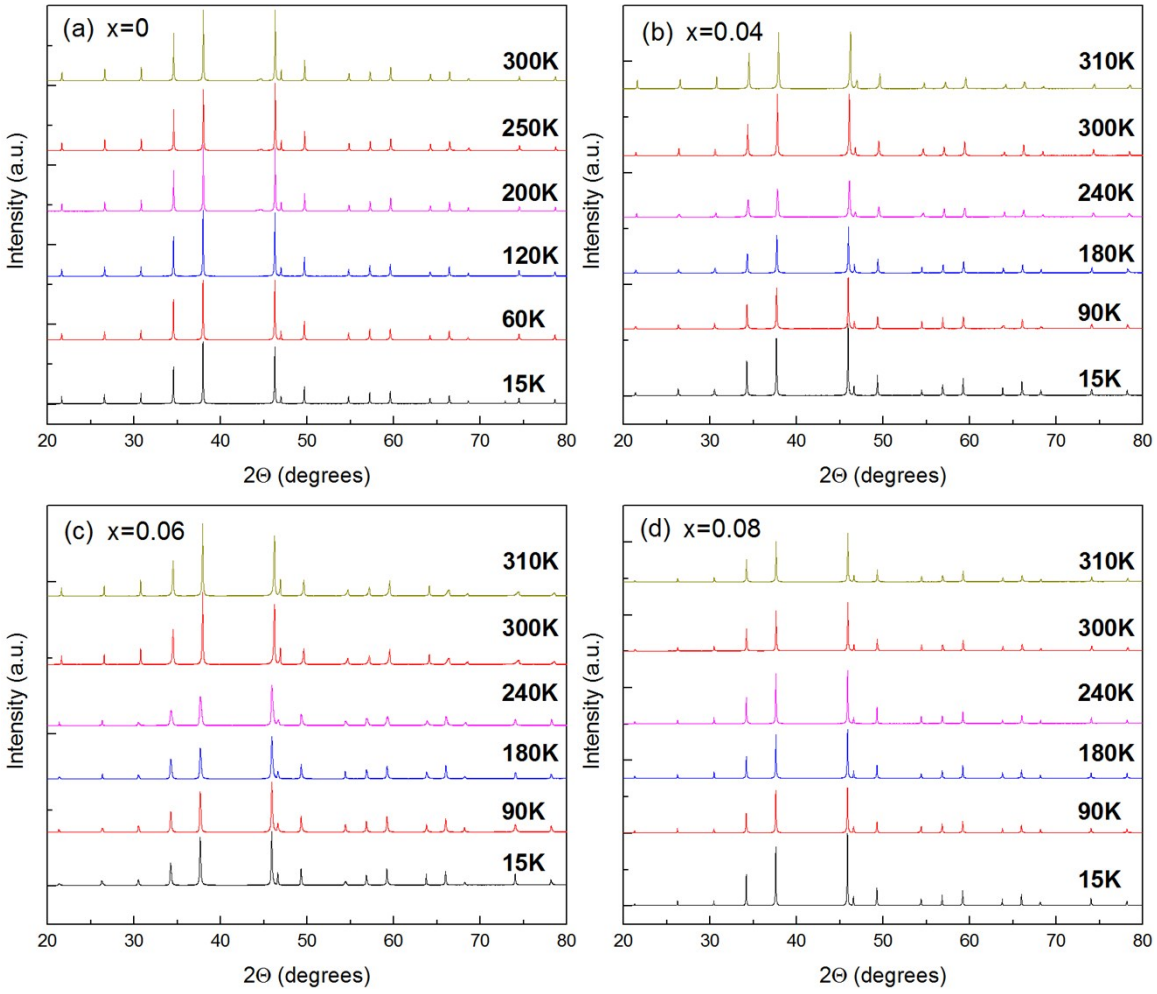

Figure S1. XRD patterns at different temperatures for samples of $La(Fe_{1-x}Co_x)_{11.4}Al_{1.6}$: a) x = 0, b) x = 0.04, c) x = 0.06 and d) x = 0.08.

To explore the crystal structure before and after the magnetic phase transition for $La(Fe_{1-x}Co_x)_{11.4}Al_{1.6}$ compounds, the variable-temperature XRD patterns for the samples were collected and are shown in Figure S1. The results demonstrate that they remain the cubic $NaZn_{13}$-type structure in the whole examined temperature range.

III. Isotherm magnetization

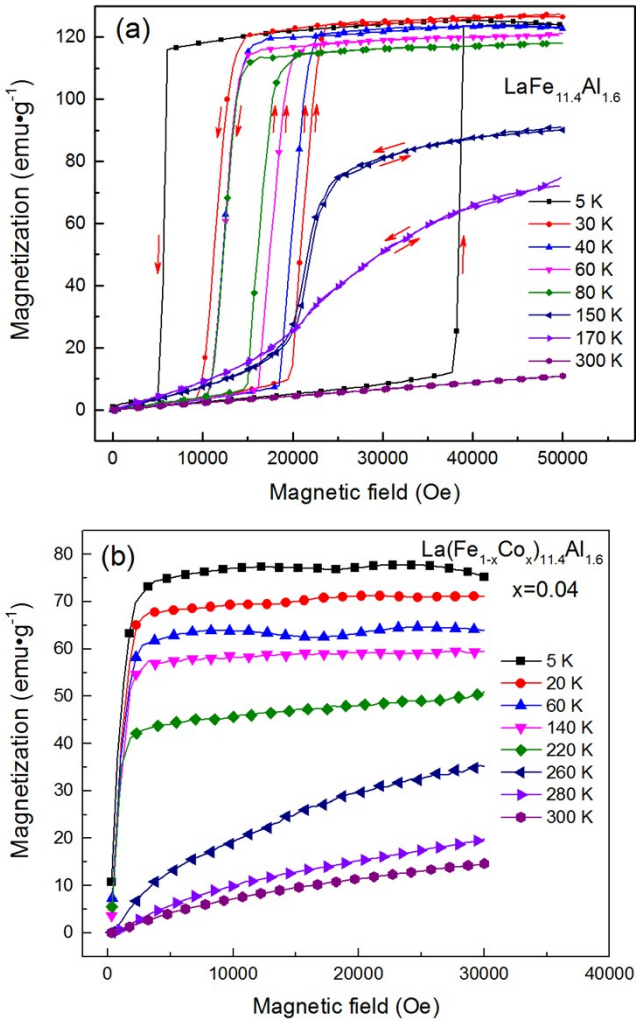

Figure S2. Isotherm magnetization *M*(*H*) curves at different temperatures for samples of $La(Fe_{1-x}Co_x)_{11.4}Al_{1.6}$: a) x = 0 and b) x = 0.04.

Isotherm magnetization *M*(*H*) curves are also measured for further understanding the relationship between magnetic properties and applied fields at different temperatures. From Figure S2(a), we can notice that the $LaFe_{11.4}Al_{1.6}$ compound shows an AFM state at low temperature, whereas the AFM ordering is weak and can be easily driven into the FM state by applying an external magnetic field. What deserve attention is the hysteresis loops around the metamagnetic transition, which become narrow with the increase of temperature,

and finally disappear at T_N. However, Figure S2(b) indicates the disappearance of antiferromagnetic order for $La(Fe_{1-x}Co_x)_{11.4}Al_{1.6}$ compounds by introducing a small amount of Co content. The results show the great effect of Co doping on the magnetic properties.

References

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