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Studying of doping boron and carbon in $LaFe_{11.6}Si_{1.4}$ magnetocaloric alloy by experimental and density-functional methods

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Abstract Both magnetic transition and magnetocaloric properties of $LaFe_{11.6}Si_{1.4}$ doped with boron (B) and carbon (C) were investigated in the present work. Experimental results showed that nearly pure $\tau 1$ phase was obtained in $LaFe_{11.6}Si_{1.4}$, $LaFe_{11.6}Si_{1.4}B_{0.06}$ and $LaFe_{11.6}Si_{1.4}C_{0.06}$ alloys after annealing at 1373 K for 100 h. All annealed samples underwent a first-order magnetic transition. B doping decreased the magnetic transition temperature from 192 K to 188 K, whereas C doping increased to 206 K. The density-functional theory assessment was used to reconstruct the unit-cell in order to understand the magnetic transition behavior. In combination with X-ray diffraction results, it was proposed that almost all B atoms occupy 96*i* FeII/Si substitutional site, and all C atoms prefer 24*d* interstitial site in the present given conditions. The annealed samples possessed the maximum magnetic entropy changes higher than 20 J/(kg·K) under a magnetic field change of 3 T, and their effective refrigeration capacities reached 200 J/kg.

Keywords: rare earth compounds; crystal structure; magnetocaloric; phase transitions; X-ray diffraction; magnetic measurements

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