

Accepted Manuscript

Studying of doping boron and carbon in $\text{LaFe}_{11.6}\text{Si}_{1.4}$ magnetocaloric alloy by experimental and density-functional methods

Yuting Dai, Yuqiang Li, Zhishuai Xu, Zhiping Luo, Ke Han, Qijie Zhai, Hongxing Zheng

PII: S0925-8388(18)32314-4

DOI: [10.1016/j.jallcom.2018.06.193](https://doi.org/10.1016/j.jallcom.2018.06.193)

Reference: JALCOM 46529

To appear in: *Journal of Alloys and Compounds*

Received Date: 1 May 2018

Revised Date: 12 June 2018

Accepted Date: 18 June 2018

Please cite this article as: Y. Dai, Y. Li, Z. Xu, Z. Luo, K. Han, Q. Zhai, H. Zheng, Studying of doping boron and carbon in $\text{LaFe}_{11.6}\text{Si}_{1.4}$ magnetocaloric alloy by experimental and density-functional methods, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.06.193.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Studying of doping boron and carbon in $\text{LaFe}_{11.6}\text{Si}_{1.4}$ magnetocaloric alloy by experimental and density-functional methods

Yuting Dai ^a, Yuqiang Li ^a, Zhishuai Xu ^b, Zhiping Luo ^c, Ke Han ^d, Qijie Zhai ^b,
Hongxing Zheng ^{a,b*}

^a *Laboratory for Microstructures, Shanghai University, Shanghai 200444, China*

^b *State Key Laboratory of Advanced Special Steel, Shanghai University, Shanghai 200444, China*

^c *Department of Chemistry and Physics, Fayetteville State University, Fayetteville, NC 28301, USA*

^d *National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA*

Abstract Both magnetic transition and magnetocaloric properties of $\text{LaFe}_{11.6}\text{Si}_{1.4}$ doped with boron (B) and carbon (C) were investigated in the present work. Experimental results showed that nearly pure γ_1 phase was obtained in $\text{LaFe}_{11.6}\text{Si}_{1.4}$, $\text{LaFe}_{11.6}\text{Si}_{1.4}\text{B}_{0.06}$ and $\text{LaFe}_{11.6}\text{Si}_{1.4}\text{C}_{0.06}$ 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 96i FeII/Si substitutional site, and all C atoms prefer 24d 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

* Corresponding author. *E-mail address:* hxzheng@shu.edu.cn (H.X. Zheng).

Download English Version:

<https://daneshyari.com/en/article/7990550>

Download Persian Version:

<https://daneshyari.com/article/7990550>

[Daneshyari.com](https://daneshyari.com)