Intermetallics 31 (2012) 186–190

Contents lists available at SciVerse ScienceDirect

Intermetallics

journal homepage: www.elsevier.com/locate/intermet

Electronic structure and Fermi surface of iron-based superconductors $R_2Fe_3Si_5$ (R = Lu;Y;Sc) from first principles

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ARTICLE INFO

Article history:
Received 2 May 2012
Received in revised form
3 July 2012
Accepted 5 July 2012
Available online 23 July 2012

Keywords:
A. Rare-earth intermetallics
A. Silicides, various
B. Electronic structure of metals and alloys
B. Superconducting properties
E. Electronic structure, calculation

ABSTRACT

Electronic structures of three superconducting rare-earth iron silicides $(Lu;Y;Sc)_2Fe_3Si_5$ and non-superconducting $Lu_2Ru_3Si_5$, adopting a tetragonal crystal structure (*P4/mnc*), have been calculated employing the full-potential local-orbital method within the density functional theory. The investigations were focused particularly on the band structures and Fermi surfaces, existing in four bands and containing rather three-dimensional electronlike and holelike sheets. They support an idea of unconventional multi-band superconductivity in these ternaries, proposed earlier by other authors for $Lu_2Fe_3Si_5$, based on heat-capacity, resistivity, electromagnetic and muon spin rotation measurements. Finally, a discussion on differences in the electronic structures between the investigated here and other common families of iron-based superconductors is carried out.

1. Introduction

Iron-based superconductors draw wide interest because of recently discovered high-temperature (high-T_C) superconducting rare-earth (oxy)pnictides, like $SmFeAsO_{1-x}F_x$ and $Sr_{1-x}Sm_xFeAsF$, reaching the highest transition temperatures, T_C, of 55 K due to doping [1]. Their crystal structures are strongly anisotropic, quasi-two-dimensional (quasi-2D), being built from negatively charged PbO-type layers of iron and non-metallic atoms as well as positively charged layers of either alkaline or rare-earth atoms. However, the first known group of superconducting rare-earth iron-based compounds is the studied here family of $R_2Fe_3Si_5$ (R = Lu;Y;Sc) [2,3]. Its members crystallize in the tetragonal structure of the $Sc_2Fe_3Si_5$ type (*P4/mnc*, space group no. 128), containing iron atoms arranged both in squares within planes perpendicular to the *c* axis and in quasi-1D chains along this axis. The iron planes are lying much closer to one another than those in the (oxy)pnictides or chalcogenides, which yields a more three-dimensional (3D) configuration. These ternary iron silicides exhibit relatively low values of $T_C \leq 6.2$ K. Nevertheless, a comparison between their electronic structures and those in high-T_C (oxy)pnictides may be useful in understanding a mechanism of superconductivity (SC) in various groups of iron-based systems.

The majority of the $R_2Fe_3Si_5$ (where R = rare-earth) series order antiferromagnetically with the magnetic moments originating only from the lanthanide R atoms [4–10], except for just investigated in this paper paramagnetic superconductors, namely $Lu_2Fe_3Si_5$ ($T_C = 6.25$ K), $Y_2Fe_3Si_5$ ($T_C = 1.68$ K), and $Sc_2Fe_3Si_5$ ($T_C = 4.46$ K) [2,3,11,12]. Interestingly, a separation between two different antiferromagnetic phases and the superconducting low-temperature phase ($T_C = 0.47$ K) occurs in $Er_2Fe_3Si_5$ [13]. Finally, $Tm_2Fe_3Si_5$ becomes under pressure a reentrant superconductor, in which the superconducting state is destroyed at the antiferromagnetic transition. This compound is significantly sensitive to applied pressure and any disorder [14–17].

Meanwhile, in $Lu_2Fe_3Si_5$ a rapid depression of T_C by magnetic impurities has being explained by the effect of screening the Fe 3d electrons (diminishing conductivity) by the *f*-electrons [18–20].

Up to now, the two-gap BCS-like superconductivity model has successfully been applied to $(Lu;Y;Sc)_2Fe_3Si_5$, yielding good agreement with the experimental data [3,21–25]. The anisotropy of their superconducting properties, anomalous upper critical fields (in $Lu_2Fe_3Si_5$), and inter-band electron scattering in the case of two weak-coupled distinct gaps opened on the whole Fermi surface (FS) sheets, indicated that they are rather quasi-2D superconductors [26–29]. Furthermore, some recent works [30–32] focused on the effect of doping by non-magnetic impurities and atomic disorder induced by the neutron irradiation, both causing a fast suppression of T_C in $Lu_2Fe_3Si_5$, have questioned the conventional (phononic) mechanism of SC in the $(Lu;Y;Sc)_2Fe_3Si_5$ family, revealing the

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http://dx.doi.org/10.1016/j.intermet.2012.07.003

significance of spin fluctuations in formation of the SC state [32]. The same effect was observed in the high-T_C (oxy)pnictides after irradiation and, hence, it might be universal for all iron-based superconductors.

In this work, we investigate by *ab initio* calculations the electronic structures of the $(Lu;Y;Sc)_2Fe_3Si_5$ superconductors and the non-superconducting isostructural $Lu_2Ru_3Si_5$ counterpart [29]. In our study, we are searching particularly for a possible relation between the FS topology and superconducting properties, in analogy to other two-gap superconductors as e.g. MgB_2 [33]. Finally, we discuss the differences occurring in the electronic structures between the rare-earth iron silicides and (oxy)pnictides or chalcogenides.

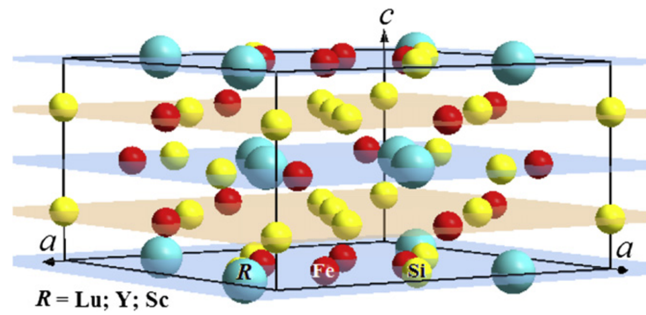

Fig. 1. Tetragonal *P4/mnc* crystal structure of the $Sc_2Fe_3Si_5$ type (no. 128).

2. Computational methods

Electronic structure calculations of $(Lu;Y;Sc)_2Fe_3Si_5$ have been performed with the full-potential local-orbital (FPLO-9) method [34]. The Perdew–Wang form [35] of the local density approximation (LDA) of an exchange-correlation functional was employed in the scalar relativistic mode. The experimental X-ray diffraction values of lattice parameters of the unit cell (u.c.) having the *P4/mnc* symmetry for $(Lu;Y;Sc)_2Fe_3Si_5$ [2] and $Lu_2Ru_3Si_5$ [36] were used as the initial ones in further optimization of the u.c. volumes by minimizing the total energy – see Table 1. Here the u.c. contains four formula units (f.u.). The crystal structure is visualized in Fig. 1 where the same experimental atomic positions as obtained for $Sc_2Fe_3Si_5$ by the single-crystal X-ray refinement [37], have been assumed for all studied here iron-based systems. This assumption is justified by the fact that isoelectronic atoms, Lu, Y, and Sc, occupy equivalent positions in the u.c. and the experimental atomic positions of the considered $Sc_2Fe_3Si_5$ system [37] and e.g. $Er_2Fe_3Si_5$ [7] differ insignificantly, in spite of a considerable disparity in size between the Sc and Er atoms. The refined experimental atomic positions of $Sc_2Fe_3Si_5$ [37] were used as follows: Sc (Y;Lu): (0.0701, 0.2500, 0); Fe(1): (0, 1/2, 1/4); Fe(2): (0.3790, 0.3601, 0); Si(1): (0.1779, 0.6779, 1/4); Si(2)): (0, 0, 0.2528); Si(3): (0.1799, 0.4761, 0). For the reference $Lu_2Ru_3Si_5$ compound, the following atomic positions were taken from the work [36]: Lu: (0.075, 0.236, 0); Ru(1): (0, 1/2, 1/4); Ru(2): (0.371, 0.356, 0); Si(1): (0.185, 0.685, 1/4); Si(2): (0, 0, 0.242); Si(3): (0.191, 0.459, 0). The valence-basis sets have been selected by automatic procedure of the FPLO-9 code. The total energy values were converged with accuracy to ~1 meV for the $16 \times 16 \times 16$ ***k***-point mesh in the Brillouin zone (BZ), containing 621 points in its irreducible wedge.

3. Results and discussion

For the $(Lu;Y;Sc)_2Fe_3Si_5$ superconductors, the optimized by the LDA computations volumes of u.c., V_{calc}, amount to about 94–95% of their experimental volumes, V_{exp}. It is worth underlining that the electronic structure results, especially the band energies and FS topology, obtained for V_{calc} are almost the same as those yielded for V_{exp}. It turned out that any further changes are also negligible when simulating even much higher pressure than that used to achieve V_{calc} starting from V_{exp}. Thus, we may assume that the large pressure effect on T_C, observed experimentally in the ternary iron silicides and reported in Ref. [38], might be

Table 1
Experimental and our calculated lattice parameters *a* and *c* (in nm) of $(Lu;Y;Sc)_2(Fe;Ru)_3Si_5$ compounds.

compound	Calculated, this paper		Experimental, Refs. [2,36]	
	a	*c*	*a*	*c*
$Lu_2Fe_3Si_5$	1.0164	0.5284	1.0340	0.5375
$Y_2Fe_3Si_5$	1.0221	0.5361	1.0430	0.5470
$Sc_2Fe_3Si_5$	1.0000	0.5257	1.0225	0.5275
$Lu_2Ru_3Si_5$	–	–	1.0611	0.5573

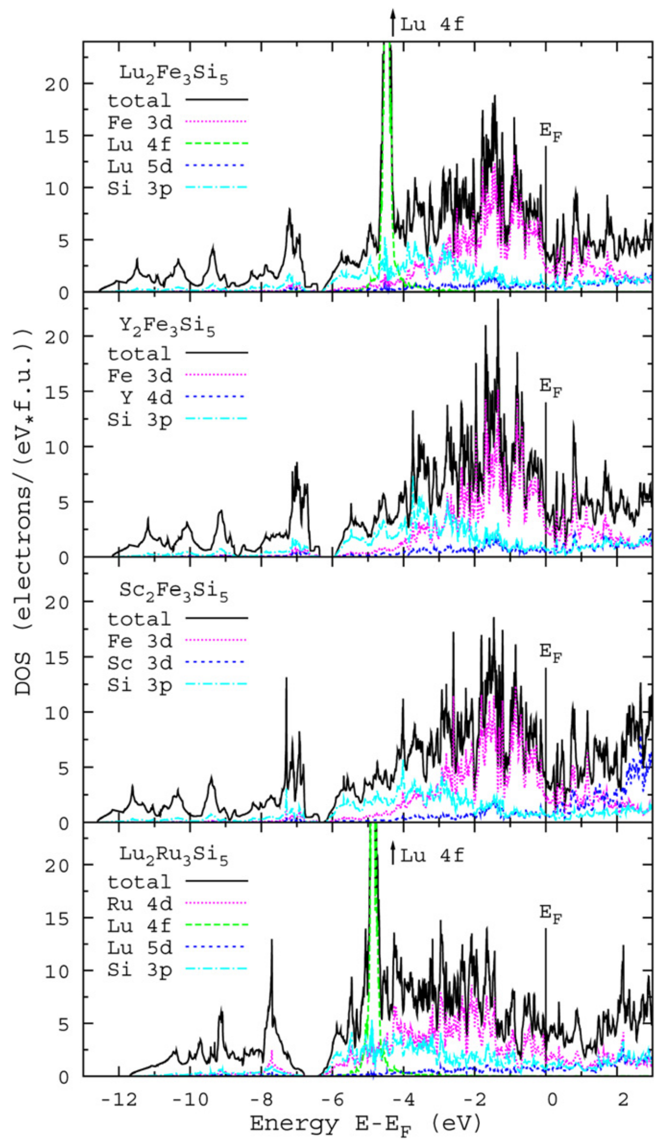

Fig. 2. Computed total and partial (per electron orbitals of transition metal, 3d/4d/5d, and other, 3p/4p, atoms) DOSs, calculated (LDA) for the $R_2Fe_3Si_5$ (R = Lu; Y; Sc) and $Lu_2Ru_3Si_5$ systems.