Entropy contribution to the stability of double perovskite $\text{Sr}_2\text{Fe}_x\text{Mo}_{2-x}\text{O}_6$

G.H. Rao$^{a,\ast}$, G.Y. Liu$^a$, X.M. Feng$^a$, Q. Zhang$^a$, J.K. Liang$^{a,b}$

$^a$Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, People’s Republic of China
$^b$International Center for Materials Physics, Chinese Academy of Sciences, Shenyang 110015, People’s Republic of China

Received 14 March 2005; revised 15 June 2005; accepted 15 June 2005
Available online 29 September 2005

Abstract

In contrast to the substitution of exotic elements such as Mn, Cu for Fe or W for Mo in $\text{Sr}_2\text{FeMoO}_6$, the degree of ordering of Fe and Mo in $\text{Sr}_2\text{Fe}_x\text{Mo}_{2-x}\text{O}_6$ shows a maximum at $x_C = 0.95$ and decreases as $x$ deviates from $x_C$. Saturation magnetization depends upon composition in a similar way. It is shown that the entropy due to antisite defects or substitutional disorder can stabilize the double perovskite structure. It is proposed that the stability of the double perovskite structure of $\text{Sr}_2\text{Fe}_x\text{Mo}_{2-x}\text{O}_6$ is essentially determined by the combined contribution to free energy of configuration entropy and differences in ionic charge and in ionic radius. A plausible charge distribution of Fe and Mo cations in $\text{Sr}_2\text{Fe}_x\text{Mo}_{2-x}\text{O}_6$ is proposed to elucidate the observed composition-dependence of magnetization.

$\copyright$ 2005 Elsevier Ltd. All rights reserved.

Keywords: Double perovskite; Cationic ordering; Stability; Configuration entropy; Magnetic moment

Sr$_2$FeMoO$_6$ has received considerable interest recently owing to the discovery of its room temperature low-field magnetoresistance (LFMR) by Kobayashi et al. [1]. The LFMR of materials is of importance both for the fundamental understanding of magnetoelectronics and for their potential applications [2]. Sr$_2$FeMoO$_6$ belongs to a double perovskite $A_2BB'_0O_6$ ($A=$Sr, Ca, Ba; $B=$Fe, Cr, Mn, etc. and $B'_0=$Mo, W, Re, etc.), in which Fe and Mo alternatively occupy the B and the $B'_0$ sites. Electronic structure calculations and optical conductivity spectrum [1,3,4] indicate that Sr$_2$FeMoO$_6$ is of half-metallic nature, i.e. the majority spin band is gapped and occupied essentially by the $3d^5$ up-spin electrons of Fe$^{3+}$ ions while the conduction band is occupied by both the Mo $4d$ $t_{2g}$ and the Fe $3d$ $t_{2g}$ down-spin electrons, leading to a full polarization of the itinerant carriers. Therefore, both the ferrimagnetic coupling between the magnetic moments of the Fe and the Mo sublattices and the metallic conductivity of the compound are induced via itinerant down-spin electrons.

The LFMR observed in Sr$_2$FeMoO$_6$ was attributed to a tunneling across grain boundaries of the spin-polarized carriers [5,6]. Within the framework of the simplest ferrimagnetic-arrangement model (the FIM model) and assuming a spin-only contribution, the moments of the Fe and the Mo sublattices are 5 and 1 $\mu_B$/f.u., respectively, for a perfectly ordered Sr$_2$FeMoO$_6$, and these sublattices couple antiferromagnetically, resulting in a saturation moment of 4 $\mu_B$/f.u. [7]. However, no perfectly ordered bulk Sr$_2$FeMoO$_6$ has been reported and antisite defects (AS), i.e. small numbers of Fe atoms on Mo sites and vice versa, were observed to exist in the compound. The reason for the incomplete ordering in Sr$_2$FeMoO$_6$ is not yet clear. Both experiments and computer simulation showed that the LFMR and the saturation moment of Sr$_2$FeMoO$_6$ are sensitive to the presence of AS [6–9]. Studies on doping the Mo site or the Fe site with exotic elements such as W, Cu, and Mn, revealed that the doping enhances the degree of B/B$'_0$ ordering, i.e. decreases the AS content [10–13]. In these systems the incidence of AS is the same in both the sublattices and changes in both simultaneously. The doping seems to expel unlike ions from each sublattice. In non-stoichiometric Sr$_2$Fe$_{x}$Mo$_{2-x}$O$_6$, mutual substitution between Fe and Mo should occur, which provides an opportunity to examine the effect of AS that inevitably presents for $x \neq 1$. 

* Corresponding author. Tel.: +86 010 82649085; fax: +86 010 82649531.
E-mail address: ghrao@aphy.iphy.ac.cn (G.H. Rao).

1468-6996/$ - see front matter $© 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.stam.2005.06.007
In addition, the valence state of Fe in Sr$_2$FeMoO$_6$ has important influence on the attractive magnetic and transport properties of the compound. Many Mössbauer spectroscopy studies have suggested two valence states for Fe. One is a mixed valence state of Fe$^{3-\delta}$ ($\delta = 0.5$) for Fe on its regular site with six Mo atoms as its nearest neighbor cations, the other is a high-spin trivalent state for Fe on a Mo site [14] or Fe on the Fe sublattice but adjacent to the nearest Mo vacancies [15] or to the antisite Fe ions [16]. However, Sleight et al. [17] and Algarabel et al. [18] observed small quadrupole splitting and argued that all Fe in Sr$_2$FeMoO$_6$ should be in high-spin trivalent state. Therefore, the valence state of Fe in Sr$_2$FeMoO$_6$ is still an open question. For non-stoichiometric Sr$_2$Fe$_{1-x}$Mo$_x$O$_6$, because of the intrinsic deficiency ($x < 1$) or excess ($x > 1$) of Fe for the Fe sublattice, any study of the cation ordering, stability and magnetic properties should be heuristic with regard to the valence state of Fe in these compounds.

Refinement results of the crystal structure of Sr$_2$Fe$_{1-x}$Mo$_x$O$_6$ have been reported in [19] and are listed in Table 1. The occupancy of Fe on the Fe site, Occ$_{Fe}$, and that of Mo on the Mo site, Occ$_{Mo}$, reach maximum values at $x = 1.0$ and $x = 0.9$, respectively. For stoichiometric Sr$_2$FeMoO$_6$, Occ$_{Fe}$ should be equal to Occ$_{Mo}$, i.e. for stoichiometric Sr$_2$FeMoO$_6$, Occ$_{Fe}$ = Occ$_{Mo}$ whereas for $x \neq 1$, Occ$_{Fe} \neq$ Occ$_{Mo}$. The degree of B/B' ordering in Sr$_2$Fe$_{1-x}$Mo$_x$O$_6$ can be defined as: $\eta = \frac{\text{Occ}_{Fe} - \text{Occ}_{Mo}}{\text{Occ}_{Fe} + \text{Occ}_{Mo}}$, where Occ$_{Fe}$ and Occ$_{Mo}$ are occupancies of Fe on the Mo site and Mo on the Fe site, respectively. The $\eta$ exhibits a maximum at $x_c = 0.95$ and is almost symmetric about $x_c$ for $0.8 \leq x \leq 1.2$. In contrast to the substitution of exotic elements such as Cu or Mn for Fe or W for Mo [10–13], the degree of B/B’ ordering in Sr$_2$Fe$_{1-x}$Mo$_x$O$_6$ decreases as $x$ deviates from $x_c = 0.95$, i.e. the substitution of Fe for Mo or Mo for Fe occurs. Reduction of the degree of B/B’ ordering by element substitution was also observed in Sr$_2$(Fe$_{1-x}$M$_x$)$_2$MoO$_6$ (M = Cr, V) [20–22]. However, Cr or V was argued to preferentially occupy the Mo site in these compounds.

It is well known that the probability for an ordered arrangement of the B, B' atoms in a double perovskite $A_2BB'O_6$ is essentially controlled by the differences between their ionic charges and between their ionic radii [23]. Therefore, the incomplete ordering in Sr$_2$FeMoO$_6$ can be due to the small difference in ionic radius between Fe$^{3+}$ and Mo$^{4+}$ ($r_{Fe}^{3+} - r_{Mo}^{4+} = 0.035$ Å, CN = 6 [24]). An occurrence of antisite defect increases the configuration entropy by $-2RT[\text{ASlnAS} + (1-\text{AS})\text{ln}(1-\text{AS})]$ and could stabilize the double perovskite structure on the one hand, where $R$ is the gas constant and $T$ is the temperature in Kelvin, but reduces the differences in average ionic radius and in ionic charge between B and B' ions and destabilizes the double perovskite structure, on the other hand. This scenario coincides with the observations that the AS in Sr$_2$FeMoO$_6$ decreases with the increasing of annealing temperature [47]. For Sr$_2$Fe(Mo$_{1-x}$W$_x$)O$_6$, the substitution of isovalent W for Mo increases the configuration entropy of the Mo

| x | Space group | a (Å) | c (Å) | Occ$_{Fe}$ | Occ$_{Mo}$ | $\eta$ |
|---|-------------|-------|-------|-----------|-----------|-------|
| 0.80 | I4/mmm | 5.5749(2) | 7.9034(5) | 0.0519(4) | 0.216(3) | 0.526(5) |
| 0.80 | I4/mmm | 5.5714(2) | 7.9007(3) | 0.0514(4) | 0.216(3) | 0.526(5) |
| 0.80 | I4/mmm | 5.5684(1) | 7.8986(2) | 0.0512(4) | 0.216(3) | 0.526(5) |
| 0.80 | I4/mmm | 5.5675(2) | 7.8962(2) | 0.0514(4) | 0.216(3) | 0.526(5) |
| 0.80 | I4/mmm | 5.5692(2) | 7.8929(2) | 0.0514(4) | 0.216(3) | 0.526(5) |
| 0.80 | I4/mmm | 5.5664(1) | 7.8898(2) | 0.0514(4) | 0.216(3) | 0.526(5) |
| 0.80 | I4/mmm | 5.5644(1) | 7.8876(1) | 0.0514(4) | 0.216(3) | 0.526(5) |
sublattice, which can partially compensate for the entropy contributed by the antisite defects, leading to a decrease of AS content, which in turn increases differences of average ionic charges and of average ionic radii between B and B’ atoms to stabilize the structure. As x increases beyond 0.5, the entropy contribution of the W-for-Mo substitution decreases. Then either the AS or differences of ionic charges and of ionic radii should increase to stabilize the double perovskite structure. Experiments have shown evidence of a valence transition of Fe from the +3 to the +2 state at x = 0.7 [11,25,26], which increases the charge difference between the cations on the Fe site and on the Mo site. The inset of Fig. 1 shows the configuration entropy based on the least-square fitted AS content reported by Kobayashi et al for Sr2Fe(Mo1–xWx)O6 [10]. At x = 0.7, the entropy decreases to that of the Sr2FeMoO6 (x = 1) with an AS content of 0.091. Therefore, the degree of ordering in Sr2FeMoO6 is essentially determined by free energy contributed by 1) the presence of AS and 2) differences in ionic charge and in ionic radius between cations on B and B’ sites. The same mechanism may be applicable to the non-stoichiometric Sr2FeMoO6 (x = 1), where x deviates from stoichiometry (x = 1), the differences in average ionic charge and in average ionic radius between B and B’ cations are reduced, but the consequent increases of antisite defects increases the entropy and stabilizes the double perovskite structure. Fig. 1 shows the configuration entropy based on the occupancies given in Table 1. The entropy exhibits a minimum at x = 0.95, which means a minimum entropy is required to stabilize the double perovskite structure in compensation for the small difference in ionic radius between Fe3+ and Mo5+. However, the differences in average ionic radius and in ionic charge between B- and B’-site ions are expected to be the largest at x = 1.0, thus the required entropy should be the minimum for this composition. When a charge distribution is taken into consideration (see below), the minimum of the entropy does occur at x = 1.0.

Since the ionic radius of Fe3+ (0.645 Å for CN = 6 [24]) is larger than that of Mo5+ (0.61 Å), the substitution of Fe3+ for Mo5+ should lead to an increase in the lattice constants. The decrease of lattice constants with x (Table 1) implies an existence of cation- or oxygen-vacancies or valence transitions of the cations. Neutron diffraction studies found no indication of antisite defects in Sr2FeMoO6 but showed evidence of cation vacancies [15,27]. The small deficiency of Mo was ascribed to the high volatility of Mo during synthesis [15], which, however, is contrary to the fact that high temperature annealing under reduced atmosphere enhances the degree of B/B’ ordering [4,7]. Oxygen vacancies in Sr2FeMoO6 were ruled out according to the coulometric titrations [14] and refinement of neutron diffraction data [15], and stoichiometry of oxygen was taken for granted in most publications [7,8,10,11]. Nevertheless, the synthesis conditions did affect the defects existing in Sr2FeMoO6 [4,7,8,15,27]. Similar defects may exist in Sr2Fe4Mo2–xO6. Since appreciable oxygen vacancies will distort the cubic perovskite structure dramatically [28], the small tetragonal distortion for x ≤ 1.2 and the crystallization of the cubic phase for x > 1.2 [19] both imply that the oxygen vacancies in Sr2Fe, Mo3–xO6 should be few in number.

Supposing that there are no cation- and oxygen-vacancies, the charge neutrality requires valence transitions of cations in non-stoichiometric Sr2FeMo2–xO6. Considering that Fe (or Mo) on the Mo (or Fe) sites in Sr2Fe,Mo2–xO6 has a local chemical environment similar to that in SrFeO3 (or SrMoO3), in which both Fe and Mo are in the +4 valence state, we propose a plausible charge distribution of cations as shown in Table 1, based on Rietveld refinement results and the charge neutrality. As presented in the table, the ions specified within the left and right pairs of parentheses occupy the Fe and Mo sites, respectively, and the other parts of the formula Sr2Fe,Mo2–xO6 are dropped for brevity. Based on the proposed charge distribution, the configuration entropy exhibits a minimum at x = 1.0, implying that the charge distribution and antisite defects stabilize the double perovskite structure of Sr2Fe4Mo2–xO6 compounds. The proposed charge distribution of cations is consistent with the response of lattice constants to the variation of composition and is reasonable from the geometric consideration, since \( r_{Fe} = 0.645 \ \text{Å}, r_{Mo} = 0.650 \ \text{Å}, r_{Fe^{4+}} = 0.585 \ \text{Å} \) and \( r_{Mo^{5+}} = 0.61 \ \text{Å} \) for CN = 6 [24]. Bond valence calculations based on the bondlengths derived from neutron powder diffraction [15,27] and single-crystal XRD data [4] give the bond valence sum of Fe on the Fe sublattice in Sr2FeMoO6 to be about 3.2 and that of Fe on the Mo sublattice to be about 3.5. The intermediate valence of Fe3+α has been revealed in cubic perovskite SrFe1–xCo2O3 by its Mössbauer spectrum [29].

![Fig. 1. Composition-dependence of configuration entropy of Sr2FeMo2–xO6 calculated based on occupancies derived from the Rietveld refinements (open circles) and the proposed charge distribution given in Table 1 (solid circles). The lines are guides to the eye. Inset: composition-dependence of configuration entropy of Sr2Fe(Mo1–xWx)O6. The unit of the entropy is in RT, where R is the gas constant and T the temperature in Kelvin.](image-url)
The saturation moment of Sr$_2$Fe$_x$Mo$_{2-x}$O$_6$ was reported by Liu et al.[30]. The composition-dependence of the saturation moment derived from the M-H curves at 4.2 K mimics that of $\eta$, exhibiting a maximum value of 3.49 $\mu_B$/f.u. at $x=0.95$. According to the FIM model and based on the proposed charge distribution, the saturation moment of Sr$_2$Fe$_x$Mo$_{2-x}$O$_6$ is estimated and shown in Table 1 and Fig. 2. The excellent agreement between the observed and the estimated moments is evidenced by the inset in Fig. 2. The data shown in Table 1 reveals that the relative deviation of the estimated saturation moment, |$M_{S,obs}^2 - M_{S,cal}^2$|/$M_{S,obs}^2$, is smaller than 4% for $x \leq 1.1$ and larger than 9% for $x \geq 1.2$ (up to 26% for $x=1.5$).

Since the possible defects in Sr$_2$Fe$_x$Mo$_{2-x}$O$_6$ have not been characterized, the proposed charge distribution of cations is tentative, though it elucidates well the composition-dependence of saturation moment and is in consistence with many observations discussed above. Other interpretations based on defects (cation- or oxygen-vacancies) cannot be excluded. Some other possible charge distributions might also comply with the measured moment within the FIM model. In addition, the FIM model is a simple mean field model that, for the sake of simplicity, omits the itinerant character of the spin-down electrons or hybridization of Fe 3$d^5$ and Mo 4$d$ t$_{2g}$ states in $\pi^*$ band [15,16]. Furthermore, when the mutual substitution is larger, i.e. $x$ deviates severely from $x=1$ and/or the antisite content AS is larger, the local chemical environment of Fe (or Mo) on Mo (or Fe) sites in Sr$_2$Fe$_x$Mo$_{2-x}$O$_6$ is obviously different from that in SrFeO$_3$ (or SrMoO$_3$), thus our proposed charge distribution may be questionable in this case. Nevertheless, the present work argues that both the configuration entropy and the differences in ionic charge and in ionic radius between cations on B and B’ sites should be taken into consideration to understand the stability of and the cationic ordering in the double perovskite compounds, which are crucial for the observed LFMR of the materials.

In summary, the degree of ordering of Fe and Mo in Sr$_2$Fe$_x$Mo$_{2-x}$O$_6$ exhibits a maximum value at $x_C=0.95$ and decreases when $x$ deviates from $x_C$, in contrast to the doping effects of exotic elements such as W, Mn, Cu. The stability of the double perovskite is essentially determined by the combined contributions to free energy of configuration entropy and differences in ionic charge and in ionic radius between cations on B and B’ sites. The saturation moment of the Sr$_2$Fe$_x$Mo$_{2-x}$O$_6$ compounds also shows a maximum value at $x_C=0.95$. A plausible charge distribution of cations is proposed to elucidate the observed composition dependence of the saturation moment within the FIM model.

The work is supported by the National Natural Science Foundation of China and by the State Key Project of Fundamental Research.

References

[1] K.I. Kobayashi, T. Kimura, H. Sawada, K. Terakura, Y. Tokura, Room-temperature magnetoresistance in an oxide material with an ordered double-perovskite structure, Nature 395 (1998) 677–680 London.
[2] G.A. Prinz, Magnetoelectronic, Science 282 (1998) 1660–1663.
[3] Y. Moritomo, Sh. Xu, A. Machida, T. Akimoto, E. Nishibori, M. Takata, M. Sakata, Electronic structure of double-perovskite transition-metal oxides, Phys. Rev. B61 (2000) R7827–R7830.
[4] Y. Tomioka, T. Okuda, Y. Akimoto, R. Kumai, K.I. Kobayashi, Y. Tokura, Magnetic and electronic properties of a single crystal of ordered double perovskite Sr$_2$FeMoO$_6$, Phys. Rev. B61 (2000) 422–427.
[5] A. Maignan, C. Martin, M. Hervieu, B. Raveau, Intragrain and intergrain magnetoresistance in Mn, Fe/Mo and Co simple, double and oxygen deficient perovskite oxides, J. Magn. Magn. Mater. 211 (2000) 173–179.
[6] D.D. Sarma, E.V. Sampathkumaran, S. Ray, R. Nagarajan, S. Majumdar, A. Kumar, G. Nalini, T.N.G. Row, Magnetoresistance in ordered and disordered double perovskite oxide MgMgO$_3$ in ordered and disordered double perovskite oxide, Sr$_2$FeMoO$_6$, Solid State Commun. 114 (2000) 465–468.
[7] L.I. Balcells, J. Navarro, M. Bibes, A. Roig, B. Martinez, J. Fontcuberta, Cationic ordering control of magnetization in Sr$_2$FeMoO$_6$ double perovskite, Appl. Phys. Lett. 78 (2001) 781–783.
[8] M. García-Hernández, J.L. Martínez, M.J. Martínez-Lope, M.T. Casais, J.A. Alonso, Finding universal correlations between cationic disorder and low field magnetoresistance in FeMo double perovskite series, Phys. Rev. Lett. 86 (2001) 2443–2446.
[9] A.S. Ogale, S.B. Ogale, R. Ramesh, T. Venkatesan, Octahedral cation site disorder effects on magnetization in double-perovskite Sr$_2$FeMoO$_6$: Monte Carlo simulation study, Appl. Phys. Lett. 75 (1999) 537–539.
[10] K.I. Kobayashi, T. Okuda, Y. Yomioka, T. Kimura, Y. Tokura, Possible percolation and magnetoresistance in ordered double perovskite alloys Sr$_2$Fe(W$_{1-x}$Mo$_x$)O$_6$, J. Magn. Magn. Mater. 218 (2000) 17–24.
[11] S. Ray, A. Kumar, S. Majumdar, E.V. Sampathkumaran, D.D. Sarma, Transport and magnetic properties of Sr$_2$FeMo$_x$W$_{1-x}$O$_6$, J. Phys.: Condens. Matter 13 (2001) 607–616.
[12] C.L. Yuan, Y. Zhu, P.P. Ong, Effect of Cu doping on the magnetoresistive behavior of double perovskite Sr$_2$FeMoO$_6$ polycrystals, J. Appl. Phys. 91 (2002) 4421–4425.
[13] X.M. Feng, G.H. Rao, G.Y. Liu, H.F. Yang, W.F. Liu, Z.W. Ouyang, L.T. Yang, Z.X. Liu, R.C. Yu, C.Q. Jin, J.K. Liang, Structure and
magnetoresistance of the double perovskite $\text{Sr}_2\text{FeMoO}_6$ doped at the Fe site, J. Phys.: Condens. Matter 14 (2002) 12503–12511.

[14] J. Lindén, T. Yamamoto, M. Karppinen, H. Yamauchi, T. Pietari, Evidence for valence fluctuation of Fe in $\text{Sr}_2\text{FeMoO}_{6-x}$ double perovskite, Appl. Phys. Lett. 76 (2000) 2925–2927.

[15] O. Chmaissem, R. Kruk, B. Dabrowski, D.E. Brown, X. Xiong X, S. Kolesnik, J.D. Jorgensen, C.W. Kimball, Structural phase transition and the electronic and magnetic properties of $\text{Sr}_2\text{FeMoO}_6$, Phys. Rev. B62 (2000) 14197–14206.

[16] J.M. Greneche, M. Venkatesan, R. Suryanarayanan, J.M.D. Coey, Mössbauer spectrometry of $\text{A}_2\text{FeMoO}_6$ (A = Ca, Sr, Ba); search for antiphase domains, Phys. Rev. B63 (2001) 174403.

[17] A.W. Sleight, J.F. Weiher, Magnetic and electrical properties of $\text{Ba}_2\text{MFeO}_6$ ordered perovskites, J. Phys. Chem. Solids 33 (1972) 679–687.

[18] P.A. Algarabel, L. Morellon, J.M. De Teresa, J. Blasco, J. García, M.R. Ibarra, T. Hernández, F. Plazaola, J.M. Barandiarán, Mössbauer spectroscopy in $\text{Sr}_2\text{FeMoO}_6$ double perovskite, J. Magn. Magn. Mater. 226-230 (2001) 1089–1091.

[19] G.Y. Liu, G.H. Rao, X.M. Feng, H.F. Yang, Z.W. Ouyang, W.F. Liu, J.K. Liang, Structural transition and atomic ordering in the non-stoichiometric double perovskite $\text{Sr}_2\text{Fe}_x\text{Mo}_{2-x}\text{O}_6$, J. Alloys Comp. 353 (2003) 42–47.

[20] J. Blasco, C. Ritter, L. Morellon, P.A. Algarabel, J.M. De Teresa, D. Serrate, J. García, M.R. Ibarra, Structural, magnetic and transport properties of $\text{Sr}_2\text{Fe}_x\text{Cr}_{2-x}\text{MoO}_{6-y}$, Solid State Sci. 4 (2002) 651–660.

[21] X.M. Feng, G.H. Rao, G.Y. Liu, H.F. Yang, W.F. Liu, Z.W. Ouyang, J.K. Liang, Effects of Cr doping on the cationic ordering and magnetic properties of $\text{Sr}_2(\text{Fe}_{1-x}\text{Cr}_x)\text{MoO}_6$, Physica B: Condens. Matter 344 (2004) 21–26.

[22] Q. Zhang, G.H. Rao, X.M. Feng, G.Y. Liu, Y.G. Xiao, Y. Zhang, J.K. Liang, Liang, Influence of V substitution for Fe on the transport and magnetic properties of $\text{Sr}_2\text{FeMoO}_6$, Solid State Commun. 133 (2005) 223–227.

[23] F. Galasso, W. Darby, Ordering of the octahedrally coordinated cation position in the perovskite structure, J. Phys. Chem. 37 (1962) 131–132.

[24] R.D. Shannon, Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides, Acta Crystallogr. A32 (1976) 751–767.

[25] T. Nakagawa, K. Yoshikawa, S. Nomura, J. Phys. Soc. Japan 27 (1969) 880–886.

[26] J. Lindén, T. Yamamoto, H. Yamauchi, M. Karppinen, Influence of W/Ta substitution at the Mo site on the Fe valence and magnetoresistive properties of $\text{Sr}_2\text{FeMoO}_6$, Physica B312-313 (2002) 787–788.

[27] C. Ritter, M.R. Ibarra, L. Morellon, J. Blasco, J. García, J.M. De Teresa, Structural and magnetic properties of double perovskites $\text{AA'}\text{FeMoO}_6$ ($\text{AA'} = $ Ba$_2$, BaSr, Sr$_2$ and Ca$_2$), J. Phys.: Condens. Matter 12 (2000) 8295–8308.

[28] T. Takeda, K. Kanno, T. Takada, O. Yamamoto, M. Takana, N. Nakayama, Y. Bando, Phase relation in the oxygen nonstoichio-metric system, $\text{SrFeO}_x$ ($2.5 \leq x \leq 3.0$), J. Solid State Chem. 63 (1986) 237–249.

[29] Maignan, C. Martin, N. Nguyen, B. Raveau, Magnetoresistance in the ferromagnetic metallic provskite $\text{SrFeO}_3$, Solid State Sci. 3 (2001) 57–63.

[30] G.Y. Liu, G.H. Rao, X.M. Feng, H.F. Yang, Z.W. Ouyang, W.F. Liu, J.K. Liang, Atomic ordering and magnetic properties of non-stoichiometric double-perovskite $\text{Sr}_2\text{Fe}_x\text{Mo}_{2-x}\text{O}_6$, J. Phys.: Condens. Matter 15 (2003) 2053–2060.