

Structural and magnetic properties of $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ nanocrystalline carbides with $0 \leq x \leq 2$

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Abstract

The crystallographic and the Curie temperature of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ ($x=0.5, 1, 1.5$ and 2) carbides have been extensively studied. X-ray diffraction studies have shown that all these alloys are approximately single phases corresponding to the $\text{Th}_2\text{Zn}_{17}$ type rhombohedral structure with a small amount of $\alpha\text{-Fe}$. The amount of this residual $\alpha\text{-Fe}$ phase decreases with increasing the Cr atomic content. It decreases from 1 wt% for $x=0.5$ to 0.4 wt.% for $x=2$. The lattice parameter c increases as a function of the Cr atomic content x from $x=0$ to $x=1.5$ and then decreases. This is due to the Cr atoms which prefer to substitute the Fe atoms in the $6c$ sites located along the c -axis. The lattice parameter a and the unit-cell volume decrease in all substitution ranges. The insertion of the C atoms leads essentially to an increase of the distances between the $9d$ and $18h$ sites and the $9d-18f$ sites. The Curie temperature reaches a maximum value of 583 K for $x=1.5$ and then decreases to 551 K for $x=2$. The enhancement of the T_c for lower Cr contents is due to a lowering of the hybridization of the iron atoms with their neighbors, the magnetovolume effect and the reduction of antiferromagnetic interactions. However, the decrease in T_c for higher Cr content is due to the reduction in the number of Fe–Fe pairs due to the magnetic dilution effect. For given interatomic distances, the exchange coupling of the Cr–Cr atoms is not of antiferromagnetic type and the exchange integral of the Cr–Cr pair is higher than that of the Fe–Fe pair.

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1. Introduction

Rare earth iron intermetallic compounds like R_2Fe_{17} have attracted much attention in recent years as possible candidates for permanent magnetic materials. Unfortunately, these binary compounds with the 2:17 structure have an easy plane magnetocrystalline anisotropy at room temperature and a remarkably low Curie temperature. It was shown that the Curie temperature can be improved by replacement of Fe by Al, Si, Ga [1] or Mn [2], but the increase is rather small. However, the insertion of interstitial carbon atoms dramatically increases the Curie temperature of the R_2Fe_{17} compounds [3]. The carbides synthesized by gas-phase interstitial reaction have poor thermal stability, thereby limiting their widespread applica-

tions [4]. Extensive studies on the substitution of non-magnetic elements such as Al, Ga at Fe site and further insertion of interstitial carbon atoms show dramatic enhancement in Curie temperature [5–7]. Also, the thermal stability of the interstitial $\text{Sm}_2\text{Fe}_{17-x}\text{M}_x$ carbides can be enhanced when $\text{M}=\text{Al}, \text{Ga}$ and Si [8–10]. A study of the effects of substitutions in the $\text{Sm}_2(\text{Fe}, \text{M})_{17}\text{C}_x$ compounds ($\text{M}=\text{Mn}, \text{Cr}, \text{V}, \text{Ti}, \text{Mo}, \text{Nb}$ and Zr) shows that $\text{Sm}_2(\text{Fe}, \text{Cr})_{17}\text{C}_x$ are the best candidates for use as permanent magnet materials [11]. The Curie temperature of $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ ($x=1, 2$ and 3) compounds decreases with increasing x despite the increase of the unit-cell volume [11]. However, the reasons of the decrease of T_c in this work was not explained. The $\text{Sm}_2(\text{Fe}, \text{Cr})_{17}\text{C}_x$ compounds obtained by arc-melting or melt spinning techniques contain a considerable amount of undesirable $\alpha\text{-Fe}$ phase [11].

This paper presents the results of structural studies performed by XRD using the Rietveld method for

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$\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ nanostructured materials. Also, the anomalous variation of the Curie temperature of these compounds has been studied.

2. Experimental details

Samples of $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ ($x=0, 0.5, 1, 1.5, 2, 2.5$ and 3) were prepared by mechanical alloying. This technique is well adapted to volatile elements with a good control of stoichiometry. This technique implies a short annealing time. The obtained nanocrystalline powders are very reactive and can easily be carburized or nitrogenated. Moreover, nanocrystalline materials give an adapted microstructure for extrinsic magnetic properties.

A mixture of high purity powders of Sm (99.99%), Cr (99.8%) and prealloyed $\text{Sm}_2\text{Fe}_{17}$ were handled inside a glove box under high purity argon gas. They were carefully weighed inside the box, in the stoichiometric ratio 2:17. The mixture was sealed in a hardened steel vial together with five 15-mm diameter steel balls. Next, the powders were ball milled in a high energy planetary ball mill, Fritsch pulverisette P7, set at intensity 10, to form an ultrafine layered microstructure. A ball to powder mass ratio of 15:1 was used with a milling time of 5 h. These milling conditions correspond to a kinetic shock energy, a shock frequency and an injected shock power, respectively, equal to 0.81 J/hit, 122 Hz and 19.5 W/g [12]. The starting $\text{Sm}_2\text{Fe}_{17}$ material is a prealloy, which will turn nanocrystalline after milling. We choose this way instead of starting from elemental powders of Sm and Fe in order to avoid oxidation.

The as-milled powder was wrapped in tantalum foil and sealed into silica tubes under a vacuum of 5×10^{-7} Torr, then they were annealed at 1425 K for 30 min. To synthesize the carbides, a given quantity of $\text{C}_{14}\text{H}_{10}$ was

added to the ball-milled alloy. The mixture was heated at 500 °C in a quartz tube under vacuum for 24 h. Some Mg pieces were put into the tube in order to absorb the hydrogen formed from the hydro-carbide decomposition. X-ray diffraction (XRD) measurements were carried out with Cu K α radiation ($\lambda=1.5405 \text{ \AA}$) on a Bruker diffractometer equipped with a single-crystal graphite monochromator. The XRD patterns were collected with and without an internal standard (silicon) to have good precision of the lattice parameter values. The data were fitted with the FULLPROF program [13] based on the Rietveld method [14]. The Curie temperatures T_c were measured in a differential sample magnetometer (Manics) in a low magnetic field of 1 kOe. T_c was determined from the $M-T$ curve by extrapolating the linear part of the $M-T$ curve and finding the temperature value of the intersection with the extended baseline.

3. Results and discussion

Fig. 1 gives the XRD patterns of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbide compounds. Based on this figure, we notice that all the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides are approximately single phases corresponding to the $\text{Th}_2\text{Zn}_{17}$ type rhombohedral structure. The crystalline peak positions of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ compounds shift to lower diffraction angles as compared to those of $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ compounds [15].

The analysis results of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ ($x=0.5, 1, 1.5$ and 2) XRD patterns, using the Rietveld method, are given in Table 1. The mean crystallite size (CS) of the synthesized $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ compounds with $x \leq 2$, obtained by fitting the XRD patterns with the Rietveld method, ranges between 350 and 400 nm. Carbides are metastable compounds and a partial decomposition into

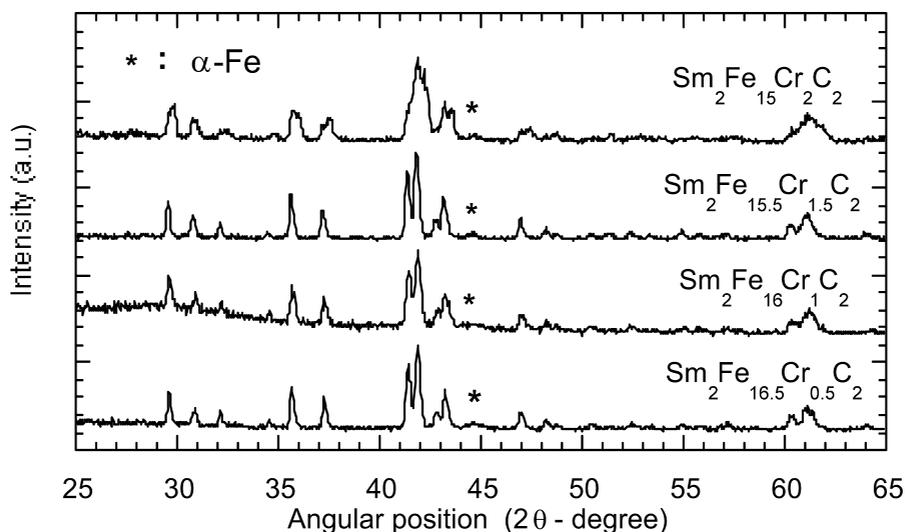


Fig. 1. XRD patterns of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides ($x=0.5, 1, 1.5$ and 2).

Table 1
XRD analysis results obtained by the Rietveld method on the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ ($x=0.5, 1, 1.5$ and 2) alloys

X	0.5		1		1.5		2	
	Alloy	Carbide	Alloy	Carbide	Alloy	Carbide	Alloy	Carbide
a (Å)	8.549	8.732	8.542	8.727	8.535	8.723	8.533	8.676
c (Å)	12.445	12.568	12.450	12.571	12.442	12.577	12.442	12.521
c/a	1.455	1.455	1.457	1.457	1.458	1.458	1.458	1.458
V (Å ³)	787.80	829.91	786.95	829.12	785.08	828.75	784.65	816.19
$\Delta V/V$ (%)	–	5.34	–	5.35	–	5.55	–	4.02
Sm, 6c, z	0.343	0.346	0.343	0.347	0.344	0.344	0.343	0.346
Fe Cr, 6c, z	0.096	0.095	0.096	0.095	0.096	0.096	0.092	0.091
Fe Cr, 18f, x	0.289	0.284	0.290	0.284	0.289	0.283	0.291	0.281
Fe Cr, 18h, x	0.502	0.505	0.502	0.506	0.501	0.506	0.501	0.504
Fe Cr, 18h, y	0.497	0.494	0.497	0.494	0.498	0.493	0.498	0.495
Fe Cr, 18h, z	0.157	0.153	0.157	0.156	0.157	0.152	0.156	0.153
%, Cr, 6c	25	25	50	50	75	75	100	100
R_B factor	6.91	5.31	5.75	6.21	4.63	6.78	4.92	5.82
R_F factor	5.79	5.76	5.03	5.44	4.06	6.44	4.49	4.29
χ^2	1.26	1.05	1.26	1.07	1.57	1.19	1.16	1.78
wt.% α -Fe	0	0.98	0	0.75	0	0.64	0	0.32

Sm/Cr carbides and soft magnetic α -Fe can take place during carburization. On the other hand, Sm/Cr carbides were not detected by the XRD measurements. It is concluded, that these carbides are in an amorphous or nearly amorphous state and they are difficult to detect by XRD. The amount of the α -Fe residual phase decreases with increasing Cr content. It decreases from nearly 1 wt.% for $x=0.5$ until 0.4 wt.% for $x=2$. It has been reported in a previous work [16] that the $\text{Sm}_2\text{Fe}_{17-x}\text{Ga}_x\text{C}_{1.5}$ compounds crystallize as a single phase with the rhombohedral $\text{Th}_2\text{Zn}_{17}$ -type structure, when x is larger than 3. It was also reported in another work [11] that contrary to the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ alloys elaborated by arc melting or melt-spinning techniques, the α -Fe crystalline peak is very intense which means that this residual phase is present in a high amount. In yet another work [1], the amount of the residual α -Fe phase when $\text{Sm}_2\text{Fe}_{16}\text{Al}$ carbides were synthesized by solid-gas reaction was almost 5 wt.%. So, mechanical alloying and the carburization mode used in this work seem to be the optimal method for the synthesis of almost pure carbides.

The analyses of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ alloys XRD patterns, using the Rietveld method, give the best values of the fit parameters R_B , R_F and χ^2 when Cr replaces the Fe atoms in the 6c sites and the C atoms in the 9e interstitial sites (Fig. 2). It has been reported in our previous work [15] that the Cr atoms prefer to occupy the 6c sites. The substitution of Cr for the Fe atoms occupying these 6c sites induces an increase of the lattice parameter c until $x=1.5$ where it reaches its maximum value of 12.577 Å. Then, it decreases until $x=2$ (Fig. 3). We suggest that the behaviour of the lattice parameter c is probably due to the anomalous character of the R_2Fe_{17} compounds as regards: thermal expansion, forced volume magnetostriction, pressure dependence of the Curie temperature and the magnetic moment formation [2].

In the whole substitution field, the lattice parameter a decreases when increasing the Cr content x (Fig. 3) in order to accommodate the lattice deformation induced by the increase of the lattice parameter c . We remark that the parameter a of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbide is higher than that of $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$. This is due to the fact that the carbon atoms prefer going into the 9e interstitial sites having (1/2, 0, 0) as coordinates and being located along the a -axis. The decrease of the unit-cell volume V , when increasing the Cr content x (Fig. 4), is due to the fact that its value is more influenced by the value of the lattice parameter a than by that of the lattice parameter c as $V = \sqrt{3}/2a^2c$. The variation of the c/a ratio with Cr content suggests that the unit cell volume compression is anisotropic.

Contrary to our results, Chen et al. [11] showed in a previous work on $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ ($x=1, 2$ and 3) that the

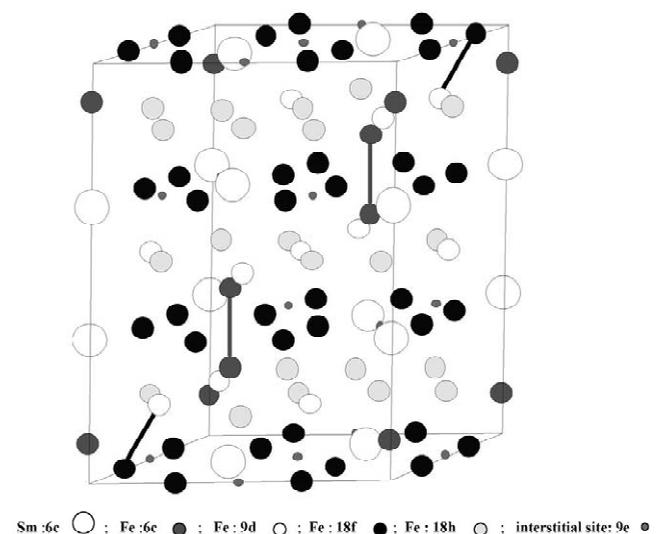


Fig. 2. Crystal structure of the $\text{Sm}_2\text{Fe}_{17}$ compound.

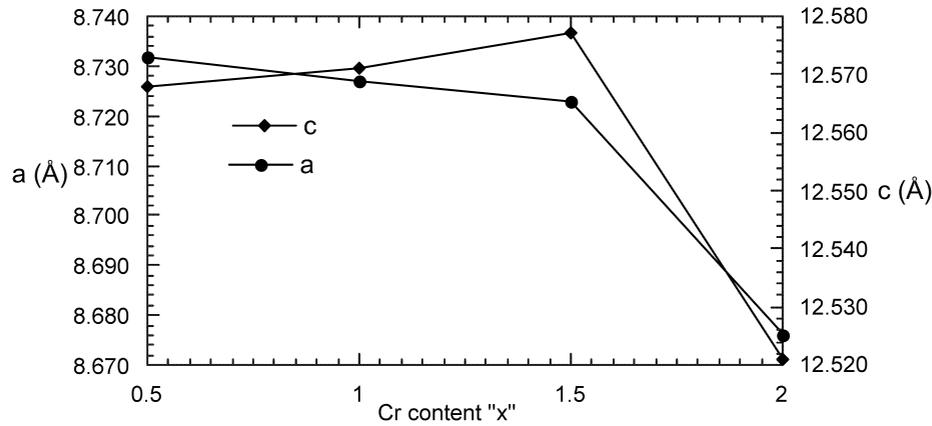


Fig. 3. Variation of the lattice parameters a and c of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides versus the Cr content x .

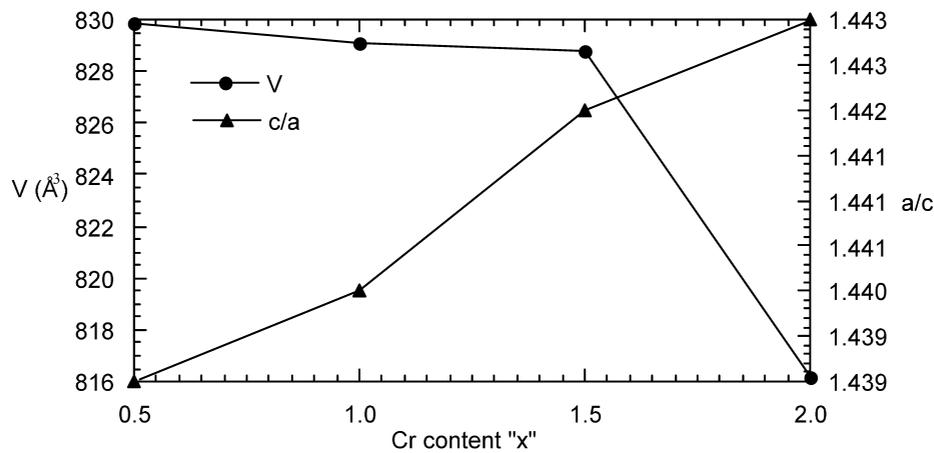


Fig. 4. Variation of the c/a ratio and unit-cell volume V of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides as a function of the Cr content x .

lattice parameters a and c and the unit cell volume V increased when increasing the Cr content x . Also, Shen et al. [16] reported the same properties for the $\text{Sm}_2\text{Fe}_{17-x}\text{Ga}_xC_{1.5}$ ($0 \leq x \leq 6$) alloys. The same authors [16] assume that this behavior is due to the fact that the Ga atoms of which the atomic radius is equal to 1.41 Å replace the Fe atoms in the $18h$ sites (the coordinates of this site position are: 0.5, 0.5, 0.167). This substitution mode differs from that reported in our work where the Cr atoms prefer to replace the Fe atoms in the $6c$ sites of which the position coordinates are: 0, 0, 0.097.

Table 2 gives the Curie temperatures of the

Table 2
The T_c of alloys $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ and their carbides

Cr content x	Alloy $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ [15]	Carbide $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$
0	417	
0.5	446	491
1	447	539
1.5	442	583
2	424	551

$\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$ carbides and the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ alloys [15]. Fig. 5 gives the variation of the Curie temperature of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$ carbides and $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ alloys [15] as a function of the Cr content x . One could remark that the Curie temperatures of the carbides increase as compared to those of the alloys with the same composition. We can explain this increase by the magneto-volume effect and the lowering of the hybridization of the iron atoms with their neighbors. In fact, the insertion of the C atoms leads to an increase of the lattice volume expansion of about 5% as compared to the non-carburized alloy having the same composition. The Curie temperature increases and reaches a maximum value of 583 K for the $\text{Sm}_2\text{Fe}_{15.5}\text{Cr}_{1.5}\text{C}_2$ carbide ($x=1.5$) despite the contraction of the unit cell volume as a function of the Cr content (Table 1), and then decreases to reach 551 K for $x=2$. A similar behavior has also been found for $\text{Sm}_2\text{Fe}_{17-x}\text{Ga}_xC_{1.5}$ where T_c increases to reach a maximum value of 633 K at $x=2$, and then decrease monotonically [16]. Chen and Hadjipanais [11] have found that the Curie temperature of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$ ($x=1, 2$ and 3) alloys decreases from 543 K for $x=1$ to 443 for $x=2$.

Fig. 6 gives the distance variation of the $6c-6c$ dumb-

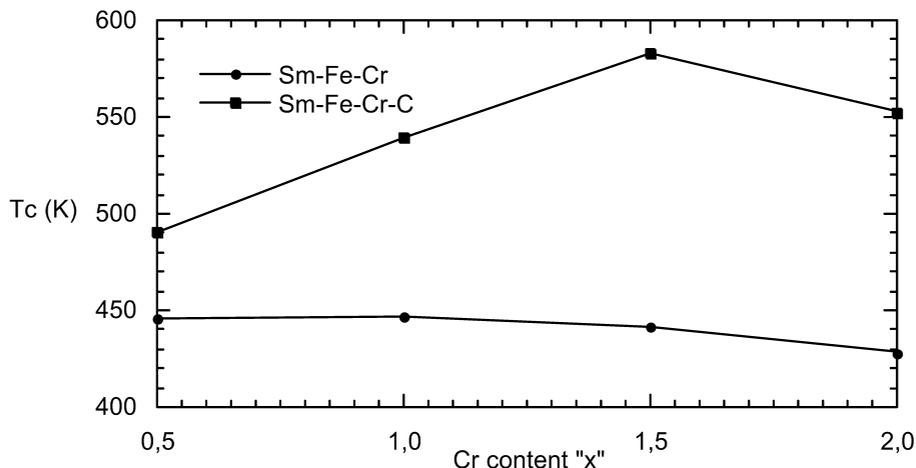


Fig. 5. Variation of the Curie temperature of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x$ alloys [15] and the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides as a function of the Cr content x .

bell sites and the $9d-18f$ sites for the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides as a function of the Cr content x . We notice that the Curie temperature T_c (Fig. 5) displays the same trend as the $6c-6c$ dumbbell site and $9d-18f$ site distances.

Based on the mean-field theory, Li and Morrish [17] have deduced the exchange integrals for $\text{Sm}_2\text{Fe}_{17}$ and $\text{Sm}_2\text{Fe}_{17}\text{N}_y$, as a function of the distance between the Fe–Fe pairs, by fitting the Mössbauer hyperfine field data at various temperatures for each Fe site. Their results [17] show that when the interatomic distance is smaller than 2.45 \AA , the exchange interactions between the Fe–Fe pairs are negative. Nevertheless, when Fe atoms are located at larger distances the interactions are positive. In the $\text{Sm}_2\text{Fe}_{17}$ lattice, as only the $\text{Fe}(6c)-\text{Fe}(6c)$ and the $\text{Fe}(9d)-\text{Fe}(18f)$ pairs have interatomic distances less than 2.45 \AA , they exhibit negative exchange integrals of, respectively, -201 and -20 K [17]. This leads to a rather low Curie temperature for the $\text{Sm}_2\text{Fe}_{17}$ compound as the latter is proportional to the J_{ij} exchange integral between the different Fe–Fe pairs [19]. For the $\text{Sm}_2\text{Fe}_{17}\text{N}_y$, the same authors [17] showed that the negative exchange

interaction between the $6c-6c$ pairs is weakened and that between the $9d-18f$ is shifted into a positive interaction. Hence, they stated [17] that the enhancement of the Curie temperature for the $\text{Sm}_2\text{Fe}_{17}\text{N}_y$ can be identified with the negative exchange interactions, a microscopic origin, instead of a volume effect, a macroscopic origin as concluded in many earlier investigations. This model well agrees with the results of Coey et al. [18].

Sabiryanov and Jaswal [19] showed that a low concentration of substitutional impurities such as Ga or Si in $\text{Sm}_2\text{Fe}_{17}$ raises its Curie temperature. Self-consistent spin-polarized electronic-structure calculations were performed and exchange parameters (J_{ij}) were derived from first-principles for pure $\text{Sm}_2\text{Fe}_{17}$ and $\text{Sm}_2\text{Fe}_{16}\text{A}$ ($\text{A}=\text{Ga}, \text{Si}$) [18]. The same authors [19] stated that the changes in exchange parameters with doping are related to the magnetovolume effect and a lowering of the hybridization of the iron atoms. In fact, the densities of states showed that both Ga and Si impurities result in a narrowing of the iron d bands which leads to an increase of the effective exchange parameter, i.e.; to a strengthening of the ex-

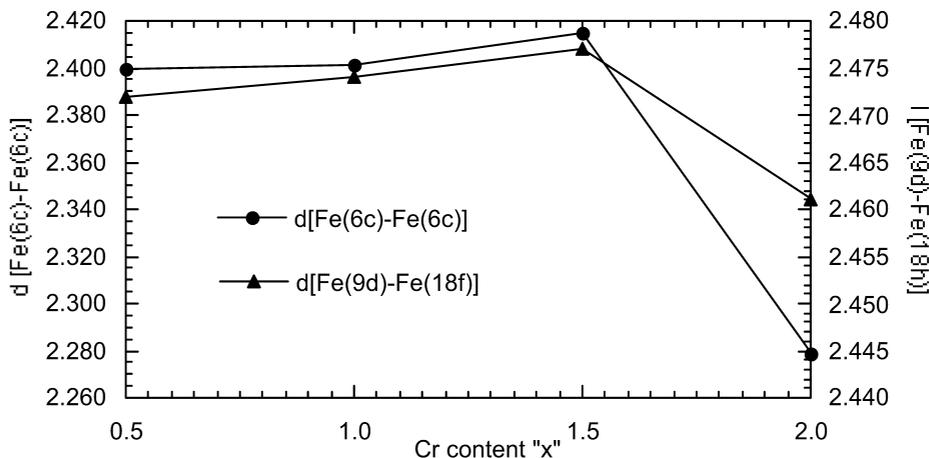


Fig. 6. Variation of the distances $d_{\text{Fe}(6c)-\text{Fe}(6c)}$ and $d_{\text{Fe}(9d)-\text{Fe}(18f)}$ of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ carbides as a function of the Cr content x .

change interactions [19]. The Monte Carlo calculations of the Curie temperatures, based on the Heisenberg model using realistic exchange parameters obtained from first principles give results which are in a good agreement with experimental data, except for the $\text{Sm}_2\text{Fe}_{17}$ phase and showed that the enhancement of the Curie temperature with doping by sp elements can be understood in terms of the lowering of the hybridization of the iron atoms with their neighbors and the magnetovolume effect [19].

So, we assume that the enhancement of the Curie temperature of $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$ carbides, when the Fe atoms were replaced by Cr atoms, can be understood as results of the lowering of the hybridization of the iron atoms with their neighbors and magnetovolume effect as stated by Sabiryanov and Jaswal [19] and Kubis et al. [1] or in terms of increase of the interatomic distances of the Fe(6c)–Fe(6c) pairs as stated by Li and Morrish [17]. In fact, apart from the fact that in the calculations of Sabiryanov and Jaswal the exchange parameters were implicitly taken into account, the effect of the interatomic distance, the variation of the Curie temperature and the interatomic distances of the Fe(6c)–Fe(6c) pairs as a function of the Cr content are in a good agreement.

Based on Table 3, for the $\text{Sm}_2\text{Fe}_{17}$ compound only the Fe(6c)–Fe(6c) and the Fe(9d)–Fe(18f) pairs have interatomic distances less than 2.45 Å and are equal, respectively, to 2.37 and 2.44 Å, corresponding to negative exchange integrals of, respectively, –201 and –20 K. These large negative values of exchange integrals are the principal cause of the low Curie temperature value of 417 K [15] obtained for this compound despite the high Fe content. In the carbides $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$, the insertion of the carbon atoms leads to an increase of the Fe–Fe distances and principally the 9d–18h and 9d–18f site distances. For the 9d–18f sites, the distance increases from 2.440 to 2.462 Å. The 6c–6c dumbbell site distance is initially indifferent to the carbon insertion but for $x=1.5$, it increases from 2.4 to 2.415 Å. For $x=1.5$, the carbide exhibits the higher Curie temperature of 583 K. We assume that this enhancement may be due to, other than the lowering of the hybridization of the iron atoms with their neighbors and magnetovolume effect, to the maximum increase of the 6c–6c (2.415 Å) and 9d–18f (2.462 Å) site distances and consequently to the increase of the total exchange integral. In fact, the interactions between these

sites become ferromagnetic and the exchange integral $J_{\text{Fe}(9d)\text{--}\text{Fe}(18f)}$ becomes positive due to the increase of the distance from 2.440 to 2.462 Å (>2.45 Å) induced by the C insertion. However, the $J_{\text{Fe}(6c)\text{--}\text{Fe}(6c)}$ increases but stays negative ($d_{\text{Fe}(6c)\text{--}\text{Fe}(6c)} < 2.45$ Å). As a consequence, the total antiferromagnetic interactions between the Fe–Fe atoms decrease.

When x becomes higher than 1.5, the dilution of the magnetic lattice by atoms whose magnetic interaction is weaker than that of Fe becomes considerable. As a result, the Curie temperature decreases to reach a value of 551 K for $x=2$. The Curie temperature of the $\text{Sm}_2\text{Fe}_{16.5}\text{Cr}_{0.5}\text{C}_2$ carbide (491 K) is less than that of the $\text{Sm}_2\text{Fe}_{15}\text{Cr}_2\text{C}_2$ carbide (551 K) despite the fact that the 6c–6c distance and the lattice volume are larger. This may prove that for $x=2$, the exchange coupling between the Cr–Cr atoms is not of antiferromagnetic type and the exchange integral of Cr–Cr pair for $d_{\text{Cr--Cr}}=2.27$ Å is higher than that of the Fe–Fe pair for $d_{\text{Fe--Fe}}=2.40$ Å ($x=0.5$).

4. Conclusion

The mechanical alloying process and the carburization mode used in this work seem to be the optimal method to synthesize pure carbides.

The XRD investigations show that the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_xC_2$ ($x=0.5, 1, 1.5$ and 2) nanostructured carbides crystallize in the $\text{Th}_2\text{Zn}_{17}$ type $R\bar{3}m$ rhombohedral structure. The quantity of the α -Fe residual phase decreases with increasing x and reaches an insignificant value of 0.32 wt.%. The lattice parameter c increases until $x=1.5$ due to the replacement of the Fe atoms by Cr atoms in the 6c sites which leads to an increase of the 6c–6c dumbbell site distance. Then it decreases until $x=2$. However, the lattice parameter a and the unit cell volume V decreases when increasing the Cr content x to accommodate the lattice deformation induced by the increase of the lattice parameter c . The insertion of the carbon atoms in the 9e interstitial sites leads to the increase of the 9d–18f site distance and consequently to the expansion of the a parameter of the carbide as compared to the alloy of same composition. The lattice volume expansion is about 5% after the insertion of the carbon atoms.

Table 3
Distance between the Fe–Fe neighbor sites

x	0		0.5		1		1.5		2	
	Alloy		Alloy	Carbide	Alloy	Carbide	Alloy	Carbide	Alloy	Carbide
6c–6c	2.377		2.401	2.400	2.404	2.401	2.402	2.415	2.299	2.279
9d–18f	2.440		2.437	2.462	2.438	2.462	2.436	2.462	2.437	2.448
9d–18h	2.474		2.451	2.526	2.449	2.523	2.456	2.525	2.456	2.510
18f–18f	2.499		2.479	2.480	2.479	2.478	2.471	2.469	2.483	2.438
18h–18h	2.485		2.521	2.544	2.515	2.533	2.502	2.545	2.499	2.528

The Curie temperature of the $\text{Sm}_2\text{Fe}_{17-x}\text{Cr}_x\text{C}_2$ compounds increases from 491 K for $x=0.5$ until 583 K for $x=1.5$, due to the increase of the total exchange integral and then decreases to reach 551 K for $x=2$, due to the magnetic dilution induced by the replacement of the strong magnetic Fe atoms by weaker magnetic Cr atoms. More attention will be paid to the $\text{Sm}_2\text{Fe}_{15.5}\text{Cr}_2\text{C}_2$ carbide, of which the Curie temperature is higher (551 K) than that of the $\text{Sm}_2\text{Fe}_{16.5}\text{Cr}_{0.5}\text{C}_2$ carbide (491 K) despite the fact that the $6c-6c$ distance and the lattice volume are smaller. This may prove that for $x=2$, the exchange coupling between the Cr–Cr atoms is not of antiferromagnetic type and the exchange integral of the Cr–Cr pair for $d_{\text{Cr-Cr}}=2.27 \text{ \AA}$ is higher than that of the Fe–Fe pair for $d_{\text{Fe-Fe}}=2.40 \text{ \AA}$ ($x=0.5$).

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