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Electronic structures and magnetic properties in $SmCo_{7-x}M_x$*

Wang Pei-Ji(王培吉)[a)b)†], Kao Hong(考 红)[c)], Zhang Chang-Wen(张昌文)[b)], Yu Feng(于 峰)[b)], and Zhou Zhong-Xiang(周忠祥)[a)]

[a)] *School of Science, Harbin Institute of Technology, Harbin* 150001, *China*
[b)] *School of Science, University of Jinan, Jinan* 250022, *China*
[c)] *Library, North China Institute of Science and Technology, Beijing* 101601, *China*

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The electronic structures and magnetic properties of $SmCo_{7-x}M_x$ (M=Ti, Si, Zr, Hf, Cu, B, Ag, Ga, Mn) compounds are investigated by using a spin-polarized MS-X.α method. The results show that the long-range ferromagnetic order is determined by a stronger 3*d*–5*d* interaction, rather than the traditional RKKY interaction, and the effects of doping element M on 3*d*–5*d* coupling are negligible in Sm–Co-based compounds. The nonmagnetic dopant Si atoms have a larger effect on the moments of 2*e* site although they preferably occupy the Co 3*g* sites, which results in the stronger uniaxial anisotropy of this compound. Analysis of the formation energies indicates that 5*d*-element doped compounds are more stable than other dopants, and furthermore, they have a higher Curie temperature above room temperature, which will be in favor of their potential application as high-temperature permanent magnets.

Keywords: electronic structure, atomic magnetic moment, exchange coupling, Curie temperature
PACC: 7500, 7115

1. Introduction

Recently, the interest has been focused on the Sm–Co intermetallic compounds with the $TbCu_7$-type structure due to their potential applications as novel high temperature permanent magnetic materials.[1−4] The $TbCu_7$ structure is a derivation of the $CaCu_5$-type structure and can be visualised as a $TbCu_5$-based compound in which 2/9 of the Tb sites are randomly replaced by dumbbell-atom pairs of Cu–Cu.[5] Experimentally, the pure binary $SmCo_7$ compound with the $TbCu_7$-type structure does not exist stably at room temperature and a third element is necessary to replace a proportion of Co in order to stabilise $SmCo_{7-x}M_x$ (M=Ti, Si, Zr, Hf, Cu, Ag, Ga, B, Mn) compounds[6−17] with the $TbCu_7$-type structure. There are three kinds of exchange couplings in Sm–Co-based compounds, i.e., Co–Co, Sm–Co and Sm–Sm couplings. From superfine field experiments, it is found that the exchange coupling between Sm–Sm atoms is negligibly small compared with those of the first two couplings. In general, the exchange coupling between Sm(4*f*)–Co(3*d*) has the same order of magnitude as that of the Co(3*d*)–Co(3*d*), but the latter gains the upper hand of the former. Some authors[18] have inferred that the polarisation effect of conductive electrons results in the exchange coupling between Sm and Co atoms. However, whether this exchange interaction of RKKY-type can produce so large a strength of coupling has always been an open problem. In order to circumvent these problems, the electronic structures and the magnetic properties of $SmCo_{7-x}M_x$ compounds are investigated in our previous paper.[19−23] Here, we attempt to address these issues. (i) What mechanism possibly leads to a long-range ferromagnetic ordering, other than RKKY interactions, in Sm–Co-based compounds? (ii) How do dopants affect the magnetic moments and the uniaxial anisotropy in these compounds? (iii) How are the formation energies and the Curie temperature of the doped Sm–Co-based compounds changed due to the lattice distortion induced by the doped elements?

MS–Xa method based on Hartree–Fock–Slater equation in energy band theory is used for studying the electronic structures and magnetic properties of crystals, where the relativistic effect is ignored.[24]

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†Corresponding author. E-mail: ss_wangpj@ujn.edu.cn

This method has been successfully applied to a wide range of polyatomic molecules and to cluster simulating local environments in crystals. The analysis of the results in Ref.[25] shows that the difference in calculation results between non-relativistic and relativistic band structure programs is about ±10%. Therefore, the error for the R–T compounds may be within ±10% when the relativistic effects are included in MS–Xa method. In order to avoid the errors arising from the $4f$ electrons, the spin-polarized MS–Xa method is used to handle Sm–Co-based clusters. It is well known that the local-spin-density approximation (LSDA)[26,27] is among the most accurate methods of performing electronic structure calculations for atoms and small molecules. However for intermetallic compounds of rare-earth and transition-metal atoms, the question whether the $4f$ states of the rare-earth metals can be considered as core states or as band states has been discussed for many years. The general trend is that the localisation of the $4f$ states is too weak in LSDA. Therefore, treating the $4f$ states as band states yields too strong a hybridisation with the other valence states, and thus the density of states at the Fermi level is much too large.[28] To obtain good results for the ground-state properties, the $4f$ states therefore were treated as core states, i.e., it is assumed that the $4f$ shell in the rare-earth metals essentially retains an atomic character determined by Hund's rules and that there are no hybridisation effects with other states. However, this model is not able to account for all aspects of rare-earth magnetism, because the correct structure of the Fermi surface may be obtained only by taking into account the hybridization between a narrow and energetically high-lying minority spin f band and the transition-metal-like valence state. This shows Sm f-orbitals are very difficult to be studied in the DFT–LSDA scheme. However, the spin-polarised MS–Xa method is well suited, in principle, for describing heavy-metal-cluster electronic structure due to a statistical approximation X_a used for the exchange–correlation potential. In the present work, we study electronic structures, exchange splittings and magnetic properties of $SmCo_{7-x}M_x$ (M=Ti, Si, Zr, Hf, Cu, Ag, Ga, B, Mn) compounds. The results presented here may be helpful not only for the understanding of substitution effects on the magnetism of $SmCo_{7-x}M_x$ compounds, but also for presenting an insight into synthesising Sm (Co, M)$_7$-series high temperature permanent magnetic materials.

2. Detail of calculation

The crystal structure of $SmCo_{7-x}M_x$ is the same as that of $TbCu_7$ ($P6/mmm$). The symmetries of Sm, Co($2c$) and Co($3g$) sites in $SmCo_{7-x}M_x$ are the same as those in Sm_5Co_{34} cluster.[23] Based on the experimental values,[6−16] the dopant Si atom prefers to occupy the $3g$ sites, while other doped atoms prefer to occupy $2e$ sites. The point group symmetries and the calculated parameters of these clusters are listed in Table 1. Due to Sm being the sixth element of lanthanum series, Sm($4f^6$) is treated as a valence orbital, and therefore we choose the valence electrons of Sm and Co atoms to be $4f^6 5s^2 5p^6 5d^0 6s^2$ and $3d^7 4s^2$, respectively. The others are treated as core electrons. Muffin-tin potentials are also used in our calculation. The partial waves with L being up to 3 for Sm and Co are included, respectively. The exchange parameter α is cited from the compilations of Schwarz.[24] The remaining parameters in the calculation are also shown in Table 1.

Table 1. Calculated parameters for $SmCo_{7-x}M_x$ compounds.

compound	$SmCo_{7-x}Ti_x$	$SmCo_{7-x}Cu_x$	$SmCo_{7-x}Hf_x$	$SmCo_{7-x}Si_x$	$SmCo_{7-x}Zr_x$	$SmCo_{7-x}B_x$	$SmCo_{7-x}Ag_x$	$SmCo_{7-x}Ga_x$	$SmCo_{7-x}Mn_x$
cluster	$Sm_5Co_{28}Ti_6$	$Sm_5Co_{30}Cu_4$	$Sm_5Co_{32}Hf_2$	$Sm_5Co_{28}Si_6$	$Sm_5Co_{32}Zr_2$	$Sm_5Co_{28}B_6$	$Sm_5Co_{32}Ag_2$	$Sm_5Co_{28}Ga_6$	$Sm_5Co_{32}Mn_2$
point group	D_{2h}	D_{2h}	C_{2h}	D_{2h}	C_{2h}	D_{2h}	C_{2h}	D_{2h}	C_{2h}
valence electrons	$3d^2 4s^2$	$3d^{10} 4s^1$	$5s^2 5p^6 5d^2 6s^2$	$3s^2 3p^2$	$4s^2 4p^6 5d^2 6s^2$	$2s^2 2p^1$	$4s^2 4p^6 4d^{10} 5s^1$	$3d^{10} 4s^2 4p^1$	$3d^5 4s^2$
L_{out}	4	5	4	5	4	4	5	5	4
radii_{MT}	0.1064 nm	0.0999 nm	0.1172 nm	0.0798 nm	0.119 nm	0.0987 nm	0.1016 nm	0.1104 nm	0.09981 nm

3. Results and discussion

The calculated results for all compounds show that the spin magnetic moments on Sm and Co atoms are antiparallel coupling to each other in $SmCo_{7-x}M_x$ compounds. The local magnetic moments of those compounds are given in Table 2, where the net spin magnetic moments on Sm in the compounds are -1.73–-0.71 μ_B in which -0.8–-1.2 μ_B is of $5d$ character. We also find that -0.1–0.17 μ_B spin moments of $6s$ electrons appear around Sm lattice, which primarily come from the spin polarisation effects of conductive electrons. Obviously, the spin moments of $5d$ electrons are parallel with those of $4f$ electrons but antiparallel with those of $6s$ electrons except for those of dopant Zr and Hf compounds. The $5d$-orbital is in the outermost shell on Sm in $SmCo_{7-x}M_x$ compounds, and therefore it is strongly extended. Thus the $5d$-orbital moment is quenched almost completely. The results also show that certain $4f$ electrons have extended characteristic to some extent, which make those $4f$ electrons very close to Fermi level. Based on magnetism theory and Hubbard model, considering the localized properties of $4f$ electrons, the orbital magnetic moments on Sm in the compounds are 2.32–4.13 μ_B. So, the atomic magnetic moments on Sm should be 1.33–1.61 μ_B in the compounds, which are in agreement with the experimental values of Sm^{3+} ion-moment (1.32–1.63 μ_B) and Sm atom-moment (1.74 μ_B) in metals.[29] The theoretical value 0.85 μ_B of Hund's rule is smaller than experimental values, for only the rather localized character of $4f$ electrons was considered, but no orbital hybridisation effects on Sm($4f^6$) and Sm($5d^0$) in the compounds were taken into account.

Table 2. Local spin, orbital, and total magnetic moments in $SmCo_{7-x}M_x$ (unit: μ_B).

compound	site	spin-moment	6*s*-spin	5*d*-spin	orbital-moment	atomic-moment	total-moment
$SmCo_{7-x}Cu_x$	Sm(1*a*)	–2.776	0.167	–1.197	4.133	1.357	9.34
	Co(2*c*)	0.72			0.493	1.213	
	Co(3*g*)	0.8575			0.420	1.2778	
	Cu(2*e*)	–0.052			–0.073	–0.125	
$SmCo_{7-x}Ti_x$	Sm(1*a*)	–1.753	0.048	–0.944	3.086	1.333	9.47
	Co(2*c*)	0.824			0.448	1.272	
	Co(3*g*)	0.894			0.603	1.497	
	Ti(2*e*)	–0.115			0.176	0.061	
$SmCo_{7-x}Si_x$	Sm(1*a*)	–1.606	0.13	–0.821	2.844	1.238	7.32
	Co(2*c*)	0.762			0.431	1.1931	
	Co(3*g*)	0.653			0.318	0.9714	
	Co(2*e*)	–0.039			–0.076	–0.1149	
$SmCo_{7-x}Zr_x$	Sm(1*a*)	–1.606	0.119	–0.83	3.017	1.411	9.95
	Co(2*c*)	1.04			0.277	1.317	
	Co(3*g*)	0.868			0.059	0.927	
	Co(2*e*)	0.105			0.179	0.284	
$SmCo_{7-x}Hf_x$	Sm(1*a*)	–1.728	–0.109	–0.834	3.059	1.331	9.98
	Co(2*c*)	0.943			0.375	1.318	
	Co(3*g*)	0.786			0.402	1.188	
	Co(2*e*)	0.145			0.137	0.282	
$SmCo_{7-x}B_x$	Sm(1*a*)	–1.501	0.12	–0.827	2.954	1.453	7.97
	Co(2*c*)	0.81			0.39	1.2	
	Co(3*g*)	0.712			0.323	1.035	
	Co(2*e*)	–0.032			–0.086	–0.118	
$SmCo_{7-x}Ag_x$	Sm(1*a*)	–1.612	0.14	–0.82	2.959	1.347	9.16
	Co(2*c*)	0.876			0.421	1.297	
	Co(3*g*)	0.732			0.353	1.085	
	Co(2*e*)	–0.037			–0.079	–0.116	
$SmCo_{7-x}Ga_x$	Sm(1*a*)	–1.589	0.12	–0.89	3.217	1.628	8.98
	Co(2*c*)	0.812			0.406	1.218	
	Co(3*g*)	0.737			0.376	1.113	
	Co(2*e*)	0.007			0.002	0.009	
$SmCo_{7-x}Mn_x$	Sm(1*a*)	–1.628	0.14	–0.85	3.154	1.526	9.01
	Co(2*c*)	0.872			0.124	0.996	
	Co(3*g*)	0.743			0.387	1.13	
	Co(2*e*)	–0.006			–0.006	–0.012	

On the other hand, we have also obtained the spin moment to be 0.65–1.04 μ_B on Co($2c$) and Co($3g$) sites, and –0.04–0.21 μ_B on $2e$ site. When a Co–Co dumbbell-atom pair replaces Sm atom, the $2e$ sites have the same interaction-surroundings as Sm site, which leads the $2e$ site to bear a negative spin moment as that of Sm does. Furthermore, the negative moments at $2e$ site decrease with the increase of M concentration. X-ray diffraction (XRD) measurements[6–13] have confirmed that $SmCo_{7-x}M_x$ compounds have a stronger uniaxial anisotropy. According to single-ion model, the magnetocrystalline anisotropy arises mainly from the contributions of the interaction between L–S coupling and crystal-field in the compounds. So, the orbital moment of $3d$ on $2e$ sites should not be quenched completely in the compounds. When the compounds are doped with different elements, we see the large effects on the magnetic moments on $2e$ site although the Si atom preferably occupied the Co $3g$ site compared with $3d$-, $4d$- or $5d$-dopants, where they occupy Co $3g$ sites,[17–20] which results in the stronger uniaxial anisotropy for Si-doped compound. Therefore, we obtain the orbital moment to be –0.6–0.28 μ_B on $2e$ site. Similarly, the orbital moments (0.06–0.46 μ_B) on $2c$ or $3g$ sites are also obtained. Thus, the total magnetic moments of $2c$ and $3g$ sites should be 0.97–1.36 μ_B, and –0.6–0.28 μ_B on $2e$ site respectively, which are smaller than those of Co in the pure metals. Reck and Fry showed that Co metal had an unquenched orbital moment of 0.147 μ_B.[30] Larson and Mazin calculated the orbital moment of Co to be 0.11–0.13 μ_B.[31] Also, the experimental values were obtained to be 0.28–0.46 μ_B in YCo_5 compound.[32,33] These results are similar to our calculated orbital moments on Co sites. Table 2 shows spin, orbital and total magnetic moments in the $SmCo_{7-x}M_x$ compounds. Obviously, the total moments of the compounds are in good agreement with the experimental values.[6–13] Compared with the case of d-doping element, however, the moments of nonmagnetic-element doped compounds are rather small, which is unfavourable for applications in practice.

As a representative for the doping Sm–Co-based compounds, the density of states (DOS) for Hf-doped compound is shown in Figs.1–4. As seen from Fig.1, we find that the number of s electrons at E_F showing the spin polarizations of conductive electrons decreases clearly as Co is partly replaced with Hf atom. The strong orbital hybridisation leads to a few of $5d$ electrons emerging around Sm atom which are mainly located at E_F and account for 4/5 of those states. The substitution effect of doping Hf results in two obvious energy gaps located at –8.0 eV and –15.1 eV separately, thereby dividing $5d$ and $4f$ electrons into three different parts. The $4f$-DOS distributes mainly below –24 eV, indicating that those $4f$ electrons are rather localised. Above the gap, the $5d$-DOS distributes mainly near E_F and has a bandwidth of about 11 eV that shows that the $5d$ electrons are more extended. For Co $3g$ sites shown in Fig.2, DOS at E_F mainly arises from d and a few of p electrons, and the number of d electrons is 7 times higher than that of p electrons. The effects of doping Hf not only make it move to E_F, but also yield one gap at –11 eV. The deep-seated DOS peaks possess the pure p-orbital character, while d-band at E_F forms ten DOS peaks, which shows that d electrons are rather extended. For Co $2c$ sites shown in Fig.3, the doping Hf leads the energy gap about 0.5 eV in $SmCo_7$ to up, and furthermore, the s-contribution to the spin-up DOS near E_F

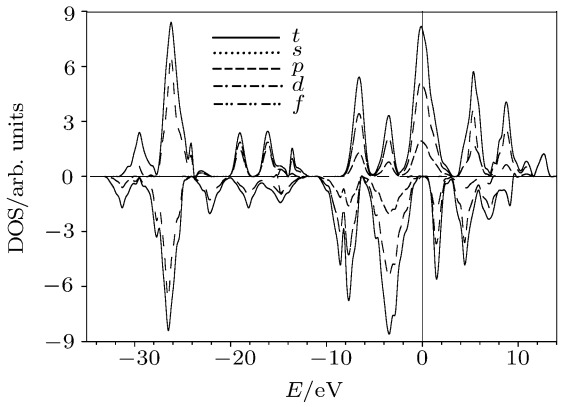


Fig.1. Density of states of Sm site in Hf-doped compound.

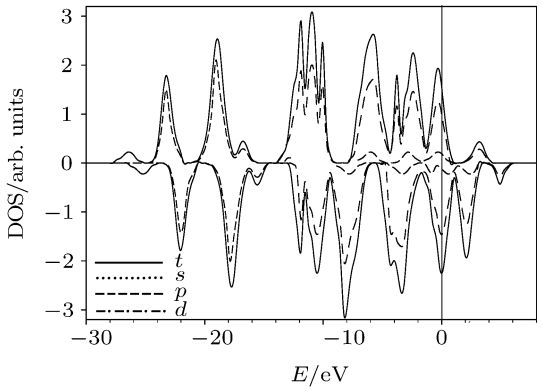


Fig.2. Density of states of $3g$ site in Hf-doped compound.

increases. Most importantly, the d-like electrons are concentrated in the vicinity of $E_{\rm F}$ and causes the negative exchange interaction to decrease distinctly, which makes the local environments of Co have the most prominent features of $SmCo_5$ as shown in Fig.4. Thus, the calculated formation energy decreases distinctively in contrast to that of $SmCo_7$, which is favourable for the stability of $SmCo_{7-x}Hf_x$.

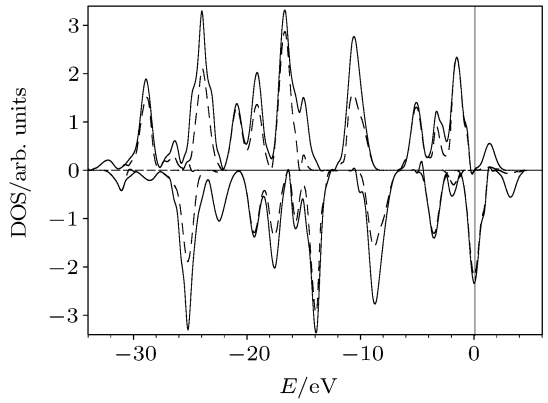


Fig.3. Density of states of 2c site in Hf-doped compound.

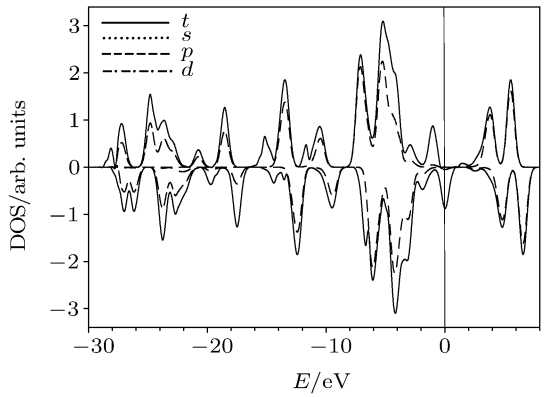


Fig.4. Density of states of 2c site in Hf-doped compound.

The hybridisation between the Co 3d and the Sm 5d states is important, in physics, for understanding the long-range magnetic properties in the Sm–Co-based compounds. When individual metals are converted into the intermetallic compounds, the hybridisation produces bonding and antibonding states, in a similar way to that for a diatomic molecule, although the states are broadened into bands here. Since the Co 3d states are lower in energy than the Sm 5d states, the dominant contribution to the antibonding states are of Co 3d nature. However, due to the hybridisation mechanism there is also spectral weight from the Sm 5d states in the antibonding orbitals, which causes a part of charges to transfer into the Sm 5d sates as shown in Table 3. Therefore, a strong coupling between Sm(5d) and Co(3d) in the vicinity of Fermi level arises, which is called 3d–5d exchange coupling. The experiments have proved that the exchange couplings between Co and Co atoms and between Sm and Co atoms determine the magnetic-ordered properties, such as Curie temperature, magnetic moment, etc. The former is a strong direct exchange interaction between 3d and 3d electrons, and the latter, which is considered, in general, to be an indirect coupling between 4f and 3d electrons, should be a weak coupling due to 4f being an inner shell of Sm. However, the superfine field experiments have found that the exchange coupling between Sm(4f) and Co(3d) atoms has the same order of magnitude as that between Co(3d) and Co(3d) atoms. Gjoka *et al* [14] inferred that the polarisation effects of conductive electrons maybe led to the stronger exchange coupling between 4f and 3d electrons. The results in the present work demonstrate that a few of s-spin moments are found around Sm and Co sites, which proves the suggestion above in a way. However, the practicability of the indirect exchange coupling of the RKKY-type for RE–TM compound is still an open problem because the polarisation effects of conductive electrons are very sensitive to the number of s electrons. When the doped M is substituted for Co atoms, we find that the Co 3d states are spin split by the intra-atomic exchange, therefore the hybridisation between the Co 3d and the Sm 5d states will be different for the two different spins. Figure 5

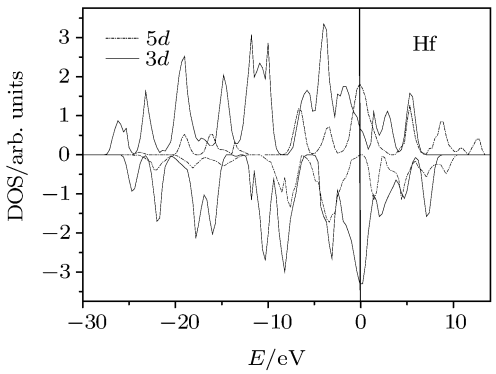


Fig.5. The 3d–5d couplings between Sm and Co atoms in $SmCo_{7-x}Hf_x$.

presents the DOS of 3d–5d couplings between Sm and Co atoms in the $SmCo_{7-x}Hf_x$ compound. It is clear that Co 3d and Sm 5d minority-spin states are closer in energy than the majority-spin states; the hybridisation is stronger for the spin-down d states than for

the majority-spin states. Hence more Sm 5*d* spin-down states will hybridize down the spin-down bonding part of the *d* complex. Independent of the type of doped elements, the stronger exchange interaction between Sm and Co atoms results in the level-splittings for 3*d* bands and 5*d* bands, and the resulting 3*d*–5*d* hybridization being stronger in minority spin, which yields the negative net spin moment. In addition, the spin directions of 3*d* and 5*d* electrons are antiparallel in doped compounds, and therefore the exchange interaction between 3*d* and 5*d* electrons should be antiferromagnetic coupling. Obviously, the 3*d*–5*d* interaction is rather stronger than the RKKY-type indirect interaction and has a similar magnitude to that of the Co–Co direct interaction in Sm–Co-based compounds. The 3*d*–5*d* interaction is intrinsic and affected little by the type and distribution of dopants, which is the main reason for the long-range ferromagnetic properties appearing in Sm–Co-based compounds. The model of 3*d*–5*d* interaction between Sm and Co atoms in Sm–Co-based compounds makes a good supplement to the problem about the exchange interaction of R–T compounds, which has been discussed for many decades already.

Table 3. Number of 5*d* electrons and the spin energy-split (unit: eV) of Co(3*d*) and Sm(5*d*) bands in $SmCo_{7-x}M_x$.

	$SmCo_7$	$SmCo_{7-x}Ti_x$	$SmCo_{7-x}Cu_x$	$SmCo_{7-x}Hf_x$	$SmCo_{7-x}Si_x$
5*d* electrons	2.886	3.648	5.625	4.794	3.323
3*d* energy-split	3.8	2.8	2.6	3.2	1.1
5*d*-energy-split	2.1	1.8	1.7	1.9	1.8
	$SmCo_{7-x}Zr_x$	$SmCo_{7-x}B_x$	$SmCo_{7-x}Ag_x$	$SmCo_{7-x}Ga_x$	$SmCo_{7-x}Mn_x$
5*d* electrons	3.774	2.871	3.456	3.765	3.358
3*d* energy-split	2.8	2.4	2.7	2.3	2.9
5*d*-energy-split	1.9	1.7	2.1	1.9	2.0

The energy splittings $[\Delta E = E_i(\downarrow) - E_i(\uparrow)]$ and the Curie temperature in all $SmCo_{7-x}M_x$ compounds are also investigated. The negative splitting levels occupy 2.82%–6.71% of the total energy levels, which leads the average exchange interaction between Co and Co atoms to decrease, resulting in a lower Curie temperature than that of pure Co metals. However, for the Cu, Ti and Si doped compounds, the negative splitting levels occupy 6.71%–6.43%, lower than metastable $SmCo_7$ phase (5.82%). Therefore the doping elements M result in the low Curie temperature for the Sm–Co-based compounds. For the Hf and Zr doped compounds, the negative splitting levels account for 2.82%–3.46%, i.e., the number of negative coupling levels decreases in the irreducible representations A_g and B_u, which makes the average exchange interaction between Co and Co atoms increase. In comparison with metastable $SmCo_7$ phase, the 5*d*-doping elements Zr and Hf would make the Curie temperature of the compounds increase up to 804 °C and 780 °C respectively, which will be in favor of their potential applications to high-temperature permanent magnets.

4. Conclusions

Using the spin-polarized MS–Xa approach we investigated the effects of doping impurity on magnetic property in all 1:7 Sm–Co based compounds. The results show that a few of electrons are transferred to $Sm(5d^0)$ orbital because of orbital hybridisation effects between Sm and Co atoms in $SmCo_{7-x}M_x$ compounds. More importantly, the 3*d*–5*d* interaction is intrinsic and affected little by the type and distribution of the dopants, which is the main reason for the long-range ferromagnetic properties appearing in Sm–Co-based compounds. The results also show that the dopant Si has the larger effects on the moments of 2*e* site although it prefers to occupy the Co 3*g* site, which results in a stronger uniaxial anisotropy of this compound. The formation energies of the compounds change in the order of $E_{SmCo5} < E_{Hf} < E_{Zr} < E_{Ga} < E_{Mn} < E_{Si} < E_B < E_{Ag} < E_{Ti} < E_{Cu} < E_{SmCo7}$, which indicates that Zr- or Hf-doped compounds should be rather stable among these

compounds. In addition, the doping Cu, Ti and Si elements will lead to the low Curie temperature, while Zr and Hf make it increase drastically, resulting in a higher Curie temperature. Therefore, we conclude that Zr- and Hf-based compounds will be in favour of their potential applications to high-temperature permanent magnets.

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