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ELECTRONIC AND MAGNETIC PROPERTIES OF $Y(FeV)_{12}$ COMPOUND AND ITS CARBIDES

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Electronic and magnetic properties of body centered tetragonal YFe_8V_4 carbon doped compounds were determined by tight-binding linear muffin-tin orbitals method assuming experimental values of lattice constants. Total, partial densities of states and magnetic moments for YFe_8V_4 and its carbides for different positions of carbon within unit cell of parent compound were calculated and discussed. In spite of carbides' unit volume decrease enhancement of magnetization and Curie temperature were obtained. Results are in quantitative agreement with experimental data.

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It has been reported that the magnetic properties of iron-rich rare-earth intermetallic compounds with $ThMn_{12}$ structure can be drastically changed upon nitrogenation or carbonation by gas-solid reaction which introduce carbon into the interstitial 2(b)-(0, 0, $\frac{1}{2}$) site [1, 2].

Recently it has been shown that some amount of carbon can be introduced into 1:12 intermetallics by arc-melting method, and the results of crystallographic and magnetic investigations of these compounds indicated that the effect of carbonation can be different from that observed in samples prepared by gas-solid method. The unit volume is observed to reduce slightly upon carbonation, and despite the unit volume reduction, saturation magnetization and Curie temperature increase significantly [3, 4]. Investigations of arc-melting $DyFe_{12-x}V_{x-y}C_y$ and $RETiFe_{12-x}C_x$ (RE = rare earth) revealed that, oppositely to the gas-solid method, carbonation causes increment of both planar magnetocrystalline anisotropy (MCA) of RE-sublattice and uniaxial MCA of 3d-sublattice [3, 5, 6]. To explain the striking magnetic behavior of the arc-melting 1:12 carbides it has been suggested that carbon may prefer to occupy other than 2(b) site, e.g. interstitial 4(d) with coordinates ($\frac{1}{2}$, 0, $\frac{1}{4}$) or substitutional site replacing one of the 3d-atom (most

probably vanadium at 8(i) sites [3, 4]. Similar occupational preference has been reported earlier for boron in $\text{RE}(\text{FeV})_{12}\text{B}$ [7] and for nitrogen in $\text{NdFe}_8\text{Co}_3\text{TiN}_{1.0}$ [8]. In view of the experimental results obtained for arc-melting 1:12 carbides it was interesting to investigate theoretically the effect of carbon placed at interstitial 4(d) and substitutional 8(i) sites and compare the results with experimental ones and with those calculated for carbon placed at 2(b) interstitial site.

In rare-earth-transition-metal (TM) intermetallic series, yttrium compounds are very convenient for studying the 3d-sublattice contribution to magnetism of $\text{RE}(\text{FeTM})_{12}$. In the paper we present the results of the self-consistent band structure calculations performed for parent YFe_8V_4 compound and its carbides. The band structure calculations were done with the use of tight-binding linear muffin tin orbital (TB-LMTO) method of Andersen [9]. We focus our attention to the dependence of electronic and magnetic properties of the carbides on crystal position (2(b), 4(d) and 8(i)) of carbon within the unit cell of reference system. For these three positions we investigated the influence of carbon on the magnetization and magnetic ordering temperature. We compare the calculated total moments and estimated Curie temperatures with the results of low temperature magnetizations measurements.

The symmetry of YFe_8V_4 structure (space group $I4/mmm$, No. 139) doped with one carbon atom depends on a position it occupies. When the 2(b) position is occupied the symmetry of the parent structure is preserved and the nearest neighbour atoms are $4 \times \text{Fe}(j)$, $2 \times \text{Y}(a)$. Single carbon atom placed into one of the 4(d) site reduces the space group to $I-4m2$ (No. 119). The nearest neighbour atoms of C at 4(d) are $4 \times \text{V}(i)$. Substitution of one of the vanadium atom at 8(i) site by carbon lowers the symmetry to orthorhombic $I2mm$ (No. 44). The number of classes of inequivalent atoms in unit cell is enlarged and the distances from C to nearest neighbour atoms increase significantly. We took the lattice parameters of carbides from experiments [4].

The resulting total densities of states (DOS) for the series of the compounds are plotted in Fig. 1. For all considered positions of carbon we observe flattening of the DOS below Fermi level (ϵ_F). In the energy region 0.8 Ry below ϵ_F there appears a non-polarized spectrum from C-2s electrons. As an effect of hybridization of 2sp-states of carbon with 3d-states of nearest neighbour TM atoms a low energy tail of DOS is truncated and the band edges become sharp. For carbon replacing vanadium atom at 8(i) site we found significant narrowing of the whole band. An influence of carbon on properties of DOS in the vicinity of Fermi level depends on its position within unit cell. The values of DOS at Fermi level are given in Table. It is noteworthy a significant lowering of $D(\epsilon_F)$ in substitutional $\text{YFe}_8\text{V}_3\text{C}$ carbide as compared to other cases.

In the carbides the way in which carbon influences the magnetic structure of parent compound is related to the position it occupies. Having analyzed the directions of local magnetic moments we found that magnetic moment of carbon orders always oppositely to the moments of its nearest neighbours. Covalent bonding of carbon at 2(b) site with nearest neighbour Fe(j) reduces the local moment of Fe(j) resulting in lowering of sample magnetization. For carbon at 4(d) site covalent bonding with nearest neighbour V(i) reduces the magnitude of the an-

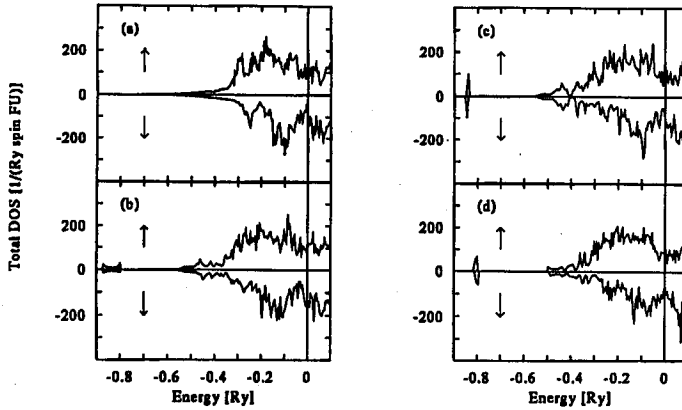


Fig. 1. Total densities of states for parent YFe_8V_4 (a), and carbides: (b) carbon at 2(b) interstitial site, (c) carbon at 4(d) interstitial site, (d) carbon at 8(i) substitutional site. Vertical line across partial pictures indicates position of the Fermi level.

TABLE

Calculated values of total densities of states at Fermi energy — $D(\varepsilon_F)$, magnetic moments per formula unit (FU) — M^{tot} , magnetic moments per Fe atom — μ_{Fe} and estimated values of Curie temperature — T_c .

	$D_{\sigma}^{\text{tot}}(\varepsilon_F)$		$D^{\text{tot}}(\varepsilon_F)$ [states/(Ry FU)]	M^{tot} [μ_B]	μ_{Fe} [μ_B/at]	T_c [K]
	$\sigma = \uparrow$	$\sigma = \downarrow$				
YFe_8V_4	123.8	70.3	194.1	10.78	1.30	300
$\text{YFe}_8\text{V}_4\text{C}$ (2b)	90.9	174.8	265.7	9.58	1.20	—
$\text{YFe}_8\text{V}_4\text{C}$ (4d)	109.5	108.7	218.2	12.99	1.62	110
$\text{YFe}_8\text{V}_3\text{C}$ (8i)	78.4	66.5	144.9	12.10	1.51	780

tiferromagnetically directed moment of vanadium giving rise to an enhancement of total magnetic moment. When carbon replaces one of vanadium atom at 8(i) site we observe enlargement of magnetization within both magnetic sublattice of Fe and V. This indicates enhancement of exchange interaction within both sublattice. This effect could be associated with the disorder caused by carbon at 8(i) site. The resulting total magnetic moments are collected in Table. The calculated magnetization per iron atom is in good quantitative agreement with experimental data ($\mu_{\text{Fe}} \approx 1.65 \mu_B$ [4]). The reduction of saturation magnetization obtained for carbide with carbon placed at 2(b) interstitial site is consistent with the results of the calculations performed for $\text{YFe}_{11}\text{TiC}$ by Qi et al. [10].

The Curie temperature (T_c) measured for YFe_8V_4 and $\text{YFe}_{12-x}\text{V}_{x-y}\text{C}_y$ is ≈ 300 K and ≈ 500 K, respectively. Having magnetization data and spin densities of states of $\text{YFe}_8\text{V}_4\text{C}$ 4(d) and $\text{YFe}_8\text{V}_3\text{C}$ carbides we estimated Curie temperature within the spin-fluctuation approximation [11] according to the formula $T_c = M_0^2 / (10k_B\chi_0)$, where $\chi_0^{-1} = (4\mu_B^2)^{-1} [N_{\uparrow}(\varepsilon_F)^{-1} + N_{\downarrow}(\varepsilon_F)^{-1}] - I/2\mu_B^2$ is the inverse exchange enhanced susceptibility, $N_{\uparrow}(\varepsilon_F)$, $N_{\downarrow}(\varepsilon_F)$ are the values of DOS at Fermi

level for up and down spin direction, respectively. We took Stoner parameter $I = 0.068$ Ry [12]. Table provides the calculated values of T_c .

On the basis of our results and estimations it can be concluded that carbides samples prepared by arc-melting method are formed as the mixture of phases with carbon placed at interstitial 4(d) sites and at substitutional 8(i) sites.

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