Spin and Orbital Moment compensation in SmAl₂. Calculations Performed with ATOMIC MATTERS MFA Computation System.

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Abstract: Crystals of SmAl₂ exhibits unusual magnetic properties in comparison to other RAl₂ (R: rare earth element), compounds reported by many authors [1-6]. Some experimental results like X-ray magnetic Compton scattering (MCS) [2], x-ray magnetic circular dichroism (XMCD)[3] reveals the decomposition of total magnetization of Sm^{3+} ions in SmAl₂ into spin and orbital contributions. We present the results of calculations of electronic and magnetic properties of SmAl₂, performed with our new computation system called ATOMIC MATTERS MFA [7-9]. A localized electron approach was applied to describe the electronic structure evolution of Sm^{3+} ions over a wide temperature range and estimate Magnetocaloric Effect (MCE) of single crystals of SmAl₂ under influence of external magnetic field applied along various directions of crystal. Magnetic and electronic properties of SmAl₂ were calculated based on the fine electronic structure of the $4f^5$ electronic configuration of the Sm^{3+} ions. Our calculations clearly confirms spin and orbital moment compensation. Our calculations yielded: magnetic moment value and direction; single-crystalline magnetization curves in zero field and in external magnetic field applied in various directions $\mathbf{m}(T,\mathbf{B}_{ext})$; the $4f$-electronic components of specific heat $c_{4f}(T,\mathbf{B}_{ext})$; and temperature dependence of the magnetic entropy and isothermal entropy change with external magnetic field $-\Delta S(T,\mathbf{B}_{ext})$. The cubic universal CEF parameters values used for definition of charge surrounding SmAl₂ was estimated: A_4=+15 Ka_0 and A_6 =-1.0 Ka_0. These studies reveal the importance of multipolar charge interactions for successive descriptions an predictions thermomagnetic properties of real $4f$ electronic systems.

Key-Words: SmAl₂, RAl₂, Laves Phase, CEF, MFA, MCE, spin-orbit coupling, Atomic Matters MFA.

1 Introduction

The RAl₂ (R: rare earth) series of compounds is fascinating by variety of different magnetic properties of their members. RAl₂ crystals have the so-called cubic Laves phase C15 structure, while the point symmetry for rare earth ions is $4\bar{3}m$. The elementary cell of the crystal structure of Laves phase is presented in fig. 1. All RAl₂ compounds are ferromagnetic, but the comparison of magnetic properties of compounds from this series compounds reveals unique magnetic properties of SmAl₂ [10].

The exotic behaviour of measured magnetic moment of Sm^{3+} ions in ordered state is the object of scientific discursion about nature of this phenomenon [1-6]. Many experimental techniques like X-ray magnetic Compton scattering (MCS) [2], x-ray magnetic circular dichroism (XMCD) [3] reveals the decomposition of total magnetization of Sm^{3+} ions into spin and orbital contributions. Significant magnetic orbital moment as well as spin is reported

in [2,3] but total magnetization measured by conventional magnetometer - based techniques, e.g., vibrating sample magnetometry (VSM) and superconducting quantum interference device magnetometry (SQUID) gives very small value of total moment m_{tot} in low temperature about ~0.2μ_B [1-6]. Samarium element is the fifth member of the $4f$-rare earth (R) series, in which spin-orbit (S-L) coupling prevails and, according to traditional description, the total angular momentum (J) governs the magnetic moment. For free Sm^{3+} ion (S=5/2, L=5, J=5/2), the $4f$-orbital contribution to the magnetic moment is 20% larger than its $4f$-spin. In crystal lattice, the degeneracy of the ground multiplet is reduced, according to interactions with electric field of crystal surrounding. Enigmatic magnetic characteristics of Sm^{3+} ions were first recognized by J. A. White and J. H. Van Vleck [1]. In early 1960's they explored a ramification of the relatively small separation between the ground J-multiplet (J = 5/2)

and the first excited state (J = 7/2). According to them changing value of total magnetic moment in the specific case of the Sm^{3+} ions is the result of the crystalline electric field CEF effect of inducing of admixture of the higher J-multiplets (J=7/2, 9/2) into the ground J-multiplet (J=5/2)[1]. Such circumstances not only substantially reduce the magnetic moment of Sm^{3+} ions, but, also make the orbital and spin contributions undergo different thermal evolutions[6]. On allowing for the admixture of higher J- multiplet into the ground J-multiplet by the perturbation of an exchange field, they could demonstrate the breakdown of the proportionality between the thermal evolution of bulk magnetic susceptibility and the local 4f-spin susceptibility as measured by the NMR Knight shifts. By applaying the Crystalline Electric Fields (CEF) to the admixture effects, that the saturation magnetic moment at Sm^{3+} vanish, with opposing orbital and spin contributions cancelling out each other.

We performed calculation of full Fine Electronic Structure of Sm^{3+} ions without perturbation methodology. The straight methodology based on intermediate CEF approach provides whole structure of multiplets of ground atomic term ^6H according to finite spin-orbit interaction in $|LSL_zS_z>$ space parametrized by spin orbit coefficient λ. In our calculations we used free ion value of $\lambda(Sm^{3+})$=350K [10]. Exchange magnetic interactions we apply according to Mean Field Approxination using self-consistent calculation methodology for molecular field calculations. This methodology makes it possible to directly simulate magnetic moment spin and orbital components. Our calculation results clearly confirm spin and orbital moment compensation in Sm ions in $SmAl_2$. We perform simulations of entropy change entropy change $-\Delta S(T,\mathbf{B}_{ext})$ for estimations of Magnetocaloric Effect (MCE) of $SmAl_2$.

The CEF (Crystal Electric Field) parameters describing the multipolar charge interaction of R ions in the crystal surrounding in this structure was agreed for all compounds from series and estimated for $SmAl_2$: A_4=+15Ka_0^{-4} and A_6 =-1.0Ka_0^{-6}..
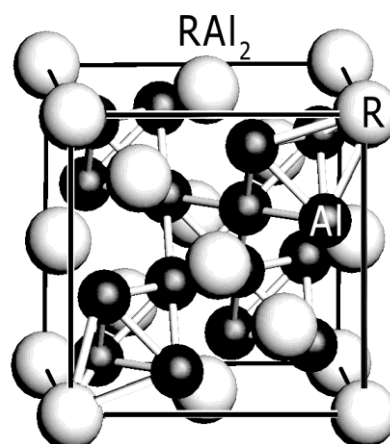

Fig.1. Cubic elementary cell of RAl_2 Laves phase C15 crystals.

2 Computation system

All calculations were performed with ATOMIC MATTERS MFA computation system. This is extension of the ATOMIC MATTERS application [7] describes fine electronic structure and predicts basic magnetic and spectral properties of materials in a paramagnetic state. ATOMIC MATTERS MFA computation system [8] provides magnetic, calorimetric and spectroscopic properties of atomic-like localized electron systems under the influence of Crystal Electric Field (CEF), spin-orbit coupling, and magnetic interactions, taken both as dynamic Mean Field Approximation (MFA), calculations and the influence of established external magnetic field $\mathbf{B}_{ext}$ [8,9]. ATOMIC MATTERS MFA provides macroscopic properties of materials in defined temperature regions, especially around the phase transition temperature: magnetic moment $\mathbf{m}(T,\mathbf{B}_{ext})$ (spin and orbital, directional components), localized electron specific heat $c_{4f}(T,\mathbf{B}_{ext})$, localized electron entropy with a useful tool set for MCE, isothermal entropy change $-\Delta S(T,\mathbf{B}_{ext})$ calculations, evolution of energy level positions, total free energy, and more. To enhance their ease of use and efficacy, both calculation systems implement an advanced Graphic User Interface (GUI) with a system of hierarchical tabs for managing calculation results, 3D interactive visualizations of potentials and fields based on Open Graphics Library (OpenGL), intuitive tools, and databases. More up-to-date information about Atomic Matters computation systems are available on our web page [9].

3 Theoretical background

Our calculation methodology is deeply rooted in atomic physics. Taking into consideration the individual population of states of fine electronic structure of ions/atoms at different temperatures according L. Boltzmann statistics makes it possible

to define the temperature dependencies of single ionic properties. According to Mean Field Approximation (MFA) methodology, magnetic phase transitions of ionic/atomic systems according to dynamic calculations of the molecular field $\mathbf{B}_{mol}$, is simply defined as:

$$\mathbf{B}_{mol}(T) = n_{mol}\mathbf{m}(T) \qquad (1)$$

Such self-consistent calculations can only be performed after establishing the molecular field factor n_{mol} that is closely related to the temperature of phase transitions, T_C.

For rapid calculations in a thermodynamically stable temperature region, ATOMIC MATTERS application offers the following CEF+Spin-Orbit+Zeeman Hamiltonian according to the chosen calculation space of ground multiplet $|J,J_z\rangle$ or ground atomic term $|LSL_zS_z\rangle$ respectively[7]:

$$H_J = H_{CEF} + H_{Zeeman} = \sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(J,J_z) + g_L \mu_B \mathbf{J} \cdot \mathbf{B}_{ext} \qquad (2)$$

or

$$H_{LS} = H_{CEF} + H_{S\text{-}O} + H_{Zeeman} =$$
$$= \sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(L,L_z) + \lambda \mathbf{L} \cdot \mathbf{S} + \mu_B(\mathbf{L} + g_e \mathbf{S}) \cdot \mathbf{B}_{ext} \qquad (3)$$

For all Hamiltonians: B_n^m denotes CEF parameters, $\mathbf{O}_n^m$ are Stevens operators, λ-is the spin–orbit constant, and g_L and $g_e \approx 2.002319$ are the gyromagnetic factors of a whole ion or single electron respectively. For a whole ion or electron respectively, μ_B is the Bohr magneton and $\mathbf{B}_{ext}$ is the external magnetic field. In all cases, calculations in the $|LSL_zS_z\rangle$ space are more physically appropriate due to their completeness, but traditional calculations with base $|JJ_z\rangle$ can be also performed by our computation systems for comparisons and rapid estimations [7,9]. For calculating properties in temperatures in ordered state and around the magnetic phase transition point, a self-consistent methodology for molecular field calculation called Mean Field Approximations (MFA) is applied. The idea behind this method is to estimate the direction and value of the magnetic field (molecular field) generated by ions at a defined temperature, and to calculate the influence of this magnetic field for electronic state structures of ions. In a selected calculation space, according to eq.1 we define a molecular field as an expected value of the total moment of the 4f electronic subshell multiplied by the molecular field, inter ionic exchange factor n_{mol}:

$$\mathbf{B}_{mol} = -n_{mol}\, g_L \mu_B \langle \mathbf{J} \rangle \qquad (4)$$

or

$$\mathbf{B}_{mol} = -n_{mol}\, \mu_B \langle \mathbf{L} + g_e \mathbf{S} \rangle \qquad (5)$$

Where the gyromagnetic factors are g_L and $g_e \approx 2.002319$. On the basis of the calculated electronic level structure $E_i(T)$, the directional

components of magnetic moments are established for all identical ions. This means that Hamiltonian matrix diagonalization is performed for all defined temperature steps recurrently. This is in contrast to simple ATOMIC MATTERS calculations [7], which diagonalize matrices one time for a single run and deduce all thermodynamic properties from the stable discrete energy level structure obtained. This self-consistent procedure provides temperature-dependent energy level structure and has one only free parameter, n_{mol}, called the molecular field parameter. The value of n_{mol} is closely related to the phase transition temperature T_C of the macroscopic structure of ions. The formal expression of the full Hamiltonian used by ATOMIC MATTERS MFA computation system, according to the chosen calculation space: $|JJ_z\rangle$ or $|LSL_zS_z\rangle$ respectively, has the form:

$$H_{J\,mol} = H_J + H_{mol} = +\sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(J,J_z) +$$
$$+ n_{mol}\, g_L^2 \mu_B^2 \left(-\mathbf{J}\langle \mathbf{J} \rangle + \frac{1}{2}\langle \mathbf{J} \rangle^2 \right) + g_L \mu_B \mathbf{J} \cdot \mathbf{B}_{ext} \qquad (6)$$

or

$$H_{LS\,mol} = \sum_n \sum_m B_n^m \hat{\mathbf{O}}_n^m(L,L_z) + \lambda \mathbf{L} \cdot \mathbf{S} +$$
$$+ n_{mol}\, \mu_B^2 \left(-(\mathbf{L} + g_e \mathbf{S})\langle \mathbf{L} + g_e \mathbf{S} \rangle + \frac{1}{2}\langle \mathbf{L} + g_e \mathbf{S} \rangle^2 \right) +$$
$$+ \mu_B(\mathbf{L} + g_e \mathbf{S}) \cdot \mathbf{B}_{ext} \qquad (7)$$

The eigenvectors of the Hamiltonian are described, according to the selected calculation base, by the total momentum quantum numbers $|JJ_z\rangle$ or spin and orbit quantum numbers $|LSL_zS_z\rangle$. Using the commutation relations of the angular momentum operators, we obtain information about expected values of the projections of magnetic momentum of all electronic states at a chosen temperature [8]:

$$m_J^\alpha(T) = \frac{g_L \mu_B}{Z(T)} \sum_i \langle J_\alpha^i \rangle \exp\left(-\frac{E_i(T)}{k_B T} \right) \qquad (8)$$

$$m_{LS}^\alpha(T) = \frac{\mu_B}{Z(T)} \sum_i \langle L_\alpha^i + g_e S_\alpha^i \rangle \exp\left(-\frac{E_i(T)}{k_B T} \right) \qquad (9)$$

Where: α indexes directional components, i numbers the Hamiltonian eigenstates, while Γ_i represents the expected value of the total angular momentum along the α-axis in the i-th state:

$$\langle J_\alpha^i \rangle = \langle \Gamma_i(T)| \mathbf{J}_\alpha | \Gamma_i(T) \rangle \qquad (10)$$
$$\langle L_\alpha^i + g_e S_\alpha^i \rangle = \langle \Gamma_i(T)| \mathbf{L}_\alpha^i + g_e \mathbf{S}_\alpha^i | \Gamma_i(T) \rangle \qquad (11)$$

All property calculations can be done for 3D (x,y,z) real space by using complex Hamiltonian matrix elements defined by full expressions of extended Stevens $\mathbf{O}_n^m$ operators. Mostly for comparison with

traditional calculation results, ATOMIC MATTERS also offers a 2D (x,z) calculation methodology of a simplified model of CEF interactions defined by Stevens O^m_n operators with real number matrix elements only [10].

Taking into consideration the possibility of the thermal population of atomic states, we automatically obtain the thermal evolution of single ion properties of the whole compound.

Under the thermodynamic principle at temperature T=0K, only the ground state is occupied. In this situation, the magnetic moment of the ion is exactly equal to the momentum of the ground state. If the temperature rises, the probability of occupying higher states increases according to Boltzmann statistics. The number of ions with energy E_i within a system at temperature T is:

$$N_i(T) = N_0 \frac{\exp\left(-\dfrac{E_i(T)}{k_B T}\right)}{Z(T)} \qquad (12)$$

where $N_0 \approx 6.022 \cdot 10^{23}$ mol^{-1} (Avogadro constant) and $Z(T)$ is the sum of states. Knowing the sum of the states, we can determine the Helmholtz free energy $F(T)$:

$$F(T) = -k_B T \ln Z(T) \qquad (13)$$

According to thermodynamic principles, the contribution of localized electrons to the total specific heat of materials can be calculated by numerical derivation of Helmholtz free energy:

$$c_{mol}(T) = -T\left(\frac{\partial^2 F(T)}{\partial T^2}\right) \qquad (14)$$

This makes it possible to calculate entropy according to the well-known definition:

$$S(T) = S(0) + \int_0^T \frac{c(T)}{T} dT \qquad (15)$$

The value of electronic entropy for a defined temperature is difficult to compare, but the isothermal change of the entropy of the system at a given temperature is a very important material parameter that describes its thermomagnetic properties. Isothermal Entropy change -$\Delta S(T, B_{ext})$, captured for different temperatures under the influence of different magnetic fields, is one the most important properties of a material that describes its usefulness as a magnetocaloric material. The value $\Delta S(T, B_{ext})$, extracted from experimental specific heat measurements, is often presented as a basic description of the Magnetocaloric Effect (MCE) of a material [12]. In our approach, isothermal entropy change can be directly calculated from eq. 15 according to the definition:

$$-\Delta S(T, B_{ext}), = S(T, B_{ext}=0)-S(T, B_{ext}). \qquad (16)$$

The exchange interactions simulated according to MFA methodology defined by eq. 1 provides simulated properties strongly dependent on the only parameter n_{mol} that is closely related to the temperature of phase transitions: T_C. It is easy to find the value of n_{mol} for correct T_C, but the value of this parameter can be estimated according to De Gennes scaling [10]:

$$T_C \sim G(f^n), \quad G(f^n) = (g_L-1)^2 J(J+1) \qquad (17)$$

De Gennes scaling is also a useful tool for n_{mol} estimation, as charge surroundings can be transferred between ions in series. The CEF part of Hamiltonian contains Stevens CEF parameters B^m_n. The values of these parameters are only appropriate for the defined ion. The recalculation of B^m_n parameters defined for an ion A in the crystal lattice surrounding of ion B in the same crystalline position follows the simple scheme:

$$B^m_n \text{ (ion A)} \rightarrow A^m_n \rightarrow B^m_n \text{ (ion B)} \qquad (18)$$

Stevens B^m_n parameters can be expressed by universal A^m_n parameters, according to the calculation space used, as follows:

$$|J,J_z\rangle; \quad B^m_n(J,J_z) = \theta_n(J) \langle r_{4f}{}^n\rangle A^m_n$$
$$|L,S,S_z,L_z\rangle; \quad B^m_n(L,L_z) = \theta_n(L) \langle r_{4f}{}^n\rangle A^m_n \qquad (19)$$

Where values of the 2nd, 4th and 6th power of average radius of a/the 4f shell $\langle r^n \rangle$ have been calculated by many authors using Hartree-Fock-type methodology, and the results can be easily found in the literature. The θ_n parameters are the J or L dependent Clebsh-Gordan-type factors, sometimes called $\alpha.\beta,\gamma$ Stevens factors $\theta_2=\alpha$, $\theta_4=\beta$, $\theta_6=\gamma$, which can be expressed by finite equations available in many papers e.g. [13]. The values of $\langle r_{4f}{}^n \rangle$ are collected in the system's open database together with references. In all presented calculations for R ions, we used the $\langle r_{4f}{}^n \rangle$ values tabulated in [13]. The ability to recalculate CEF parameters between ions and calculation spaces offers a unique chance to establish an acceptable simplification of methodology. The recalculation of CEF parameters in Atomic Matters systems is fully automated, but an explicit Stevens Factors Calculator is also available.

4 Calculation results

The CEF (Crystal Electric Field) parameters describing the multipolar charge interaction of ions in the crystal structure. The local symmetry of coordinating charges of R ion defines number of non-zero CEF parameters In case of cubic crystal field,

there is 2 only non-zero CEF parameters describing coordinating potential. The relation between cubic CEF parameters B_4 and B_6 and generally defined CEF parameters used in Hamiltonians eq.2, eq.3, eq.6 and eq.7 is simple:

$$B_4 = B_4^0 + 5B_4^0, \quad B_6 = B_6^0 - 21B_6^4 \qquad (21)$$

Universal A_n^m parameters, closely related to B_n^m was agreed for all compounds from series [11]. CEF parameters with corresponding references, established for most RAl$_2$ compounds are collected in table 1. We tested various combinations of values of A_n^m from range covering all span of values from tab.1: A_4: 5.0..23 Ka$_0^{-4}$ and A_6: -0.3..-1.1 Ka$_0^{-4}$ and we always obtained the same simulated magnetic characteristics of Sm ions in defined CEF. The value of CEF parameters for SmAl$_2$ was finally estimated according to RAl$_2$ lattice constants comparison: $A_4 = +15$Ka$_0^{-4}$ and $A_6 = -1.0$Ka$_0^{-6}$.

RAl$_2$	f^n	|JJz⟩		|LSLzSz⟩		universal		
R ion		B_4 (meV)	B_6 (meV)	B_4 (K)	B_6 (K)	A_4 (Ka$_0^{-4}$)	A_6 (Ka$_0^{-6}$)	Ref.
Pr	f^2	-4.40E-03	-8.80E-05	-5.10E-02	-1.02E-03	20.84	-0.912	11
Nd	f^3	-1.00E-03	4.00E-05	-1.16E-02	4.62E-04	13.69	-0.81	11
Sm	f^5	1.16E-04	2.24E-05	1.30E-02	2.60E-04	15	-1	(-)
Tb	f^8	3.00E-04	2.50E-07	3.48E-03	2.92E-06	17.2	-0.38	11
Dy	f^9	6.4E-05	-6.50E-07	6.50E-06	-6.38E-04	7.164	-1.038	12
Ho	f^{10}	-6.90E-05	6.40E-07	-7.99E-04	7.40E-06	17.4	-1.06	11
Er	f^{11}	1.10E-04	-1.30E-06	1.28E-03	-1.06E-05	22.63	-1.51	11

Tab1. The value of Cubic CEF parameters for RAl$_2$ series recalculated for \|LS,L$_z$,S$_z$⟩ and \|J,J$_z$⟩ space and related universal A_n^m parameters.

The spin and orbital magnetic moments of the Sm ion under condition of defined CEF are found always antiparallel coupled and the magnitude of its orbital magnetic moment is always larger than that of spin one. Calculations of electronic states in paramagnetic state (ATOMIC MATTERS methodology) reveals this antiparallel coupling between spin and orbital momentum. The full structure of energy levels in paramagnetic state, calculate in \|LS,L$_z$,S$_z$⟩ space, together with expected values of angular momentum (spin and orbital) of particular states is shown on fig.2.
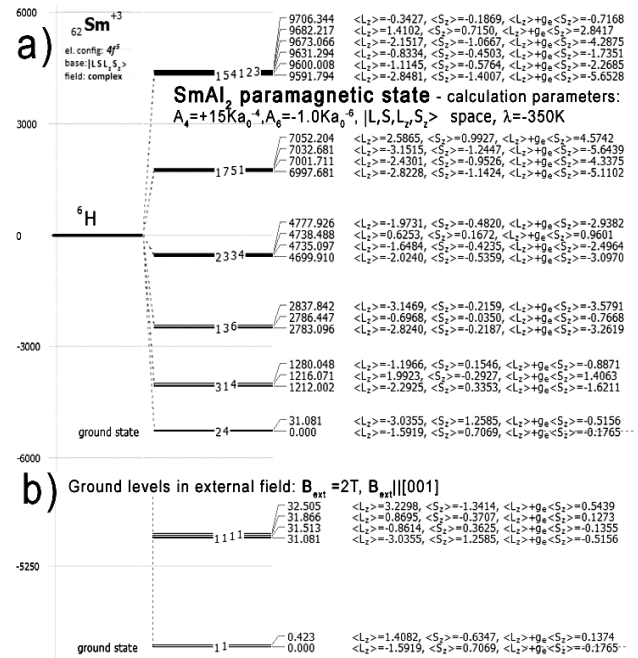

Fig.2. a) Energy level structure of Sm^{3+} ion E_i(K), under influence of defined CEF of SmAl$_2$ calculated in \|LS,L$_z$,S$_z$⟩ space. b) Lowest state of this structure, calculated uder influence of external magnetic field B_{ext}=2T applied along [001].

Obtained electronic structure clearly demonstrate spin and orbital compensation of expected values of spin and orbital component of total angular momentum.

Calculations of energy levels structure according to MFA methodology, in simplified \|J,Jz⟩ space, according to eq.6 (ground J-multiplet only) provides primitive energy levels structure shown on Fig.3. According to described methodology we calculated the total moment **m**(T) under influence of molecular field, Fig.3. To achieve Curie Temperature T_C about 120K the value of molecular field huge value was estimated of about n_{mol}=950T/μ_B. We do not have an explanation of reason of so big value of n_{mol}. Achieved that way value of ordered moment at T=0K, m(0)=0.73μ_B is more than twice big than experimental (VXM) value m$_{exp}$= 0.2μ_B [1-6]
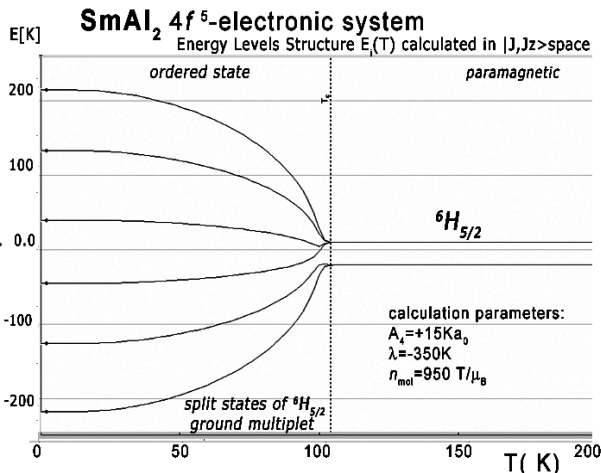
Fig.3. Ground multiplet energy levels structure vs. temperature calculated for $4f^5$ electronic system of Sm^{3+} in $SmAl_2$ calculated in $|J,Jz>$ space.
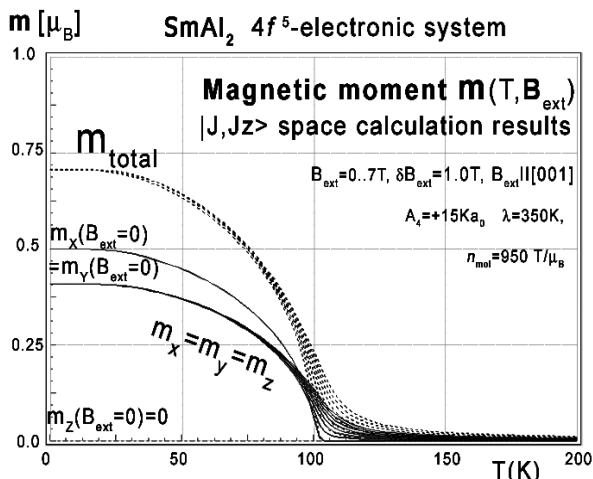

Fig. 4. Calculated x,y,z-directional components of total magnetic moment vs. temperature, calculated for for $4f^5$ electronic system of Sm^{3+} in $SmAl_2$ calculated in $|J,Jz>$ space.

The energy levels structure makes it possible to calculate localized electron specific heat under the influence of an external magnetic field, fig. 5.
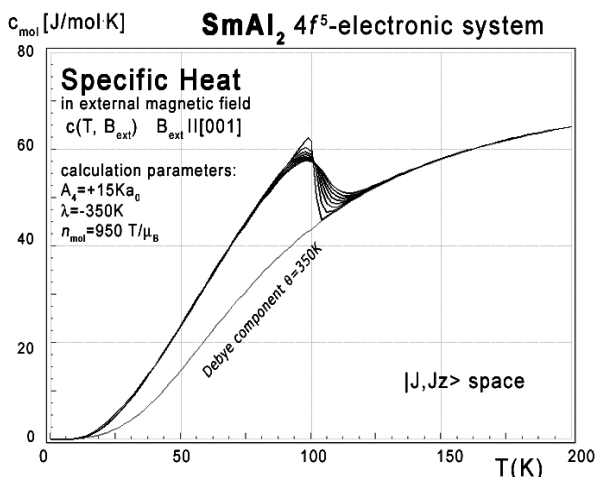

Fig. 5. Calculated $4f$-electron component of molar specific heat (eq.14) with Debye crystal lattice component (θ=350K) vs. temperature for Sm^{3+} ions in $SmAl_2$, under the influence of an external magnetic field applied along direction [001].

Collected data of specific heat makes it possible to calculate isothermal entropy change $-\Delta S(T, B_{ext})$ according to eq.16, the same methodology as used by experimentalist [12]. Isothermal entropy changes calculated with different values external magnetic fields applied along [001] direction of the cubic structure are presented on fig.6.
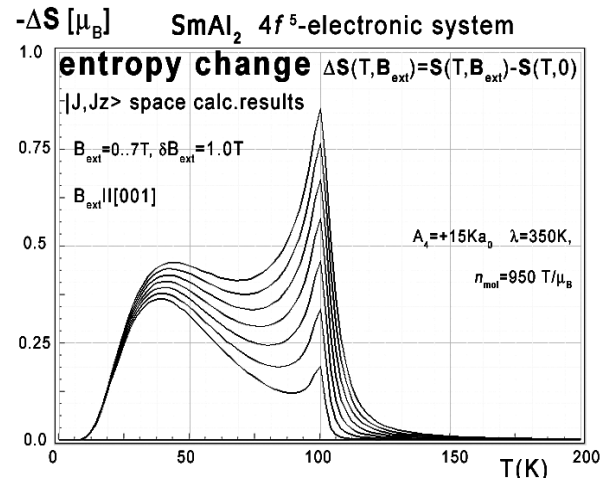

Fig.6. Calculated isothermal entropy change of $4f$-electronic system vs. temperature (eq.16) of Sm^{3+} ions in $SmAl_2$, under the influence of an external magnetic field ftom 0 to 7T applied along direction [001].
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Calculations of energy levels structure according to MFA methodology, in full $|LS,L_z,S_z>$ space, performed according to the same methodology do not provides expected effect. In every case of calculation of magnetic properties of compounds from RAl_2 series collected in Tab.1, the calculation results obtained in $|LS,L_z,S_z>$ space was better agreed with experiment and generally more valuable than perfoemed in simplified, but still conventional $|J,Jz>$ space. In the case of $SmAl_2$, calculation according to MFA methodology in $|LS,L_z,S_z>$ do not provides orderered state at all. Even using huge, unphysical values of $n_{mol}>1000T/\mu_B$ cannot force the system to ordering. It is possible another mechanism of magnetism coupling in $SmAl_2$ which cannot be simulated by simple MFA methodology defined by eq.5. Possible mechanism of ordering involves spins or orbital moments separately. In such simulations ordered moment about ~$0.2\mu_B$ is easy to obtain, but scientific correctness of such methodology needs

more experimental evidences. The simulation of energy levels structure of Sm^{3+} ions in $SmAl_2$ for orbital–only ordering mechanism is shown on fig.7.
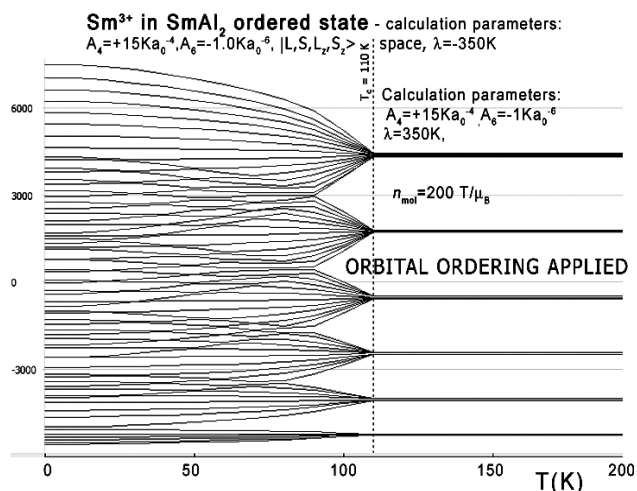

Fig.7. The result of calculations of energy levels structure vs. temperature $4f^5$ electronic system of Sm^{3+} in $SmAl_2$ calculated according to orbital coupling in $|LS,L_z,S_z>$ space.

5 Conclusions

We performed calculations for $SmAl_2$ electronic and magnetic properties using the ATOMIC MATTERS MFA computation system. The local symmetry of the Sm ions is cubic, which significantly simplifies the analyses and gives chance to evaluate calculation methodology itself. Very good agreement of obtained magnetic properties and experimental data confirms the effectiveness of our theoretical approach. Working with ATOMIC MATTERS MFA revealed its high usefulness. The visual form of calculationresults, full 3D interactive CEF potential visualization, intuitive tools for convention and unit recalculation, and the ability to compare data results all allow the user to utilize the power of the application very effectively. In conclusion, we confirm that ATOMIC MATTERS MFA is a unique application that combines a package of tools for correctly describing the physical properties of atomic-like electron systems subjected to electromagnetic interactions in real materials. This is an accurate tool for calculating properties of ions under the influence of the electrostatic potential of definable symmetry and both external and inter-ionic magnetic fields taken as a mean field approximation in magnetically ordered state. This paper is our 4th in a series devoted to the RAl_2 (R=rare earth) compounds family.

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