Interrelation of Magnetic Properties with the Crystal Structures of MeFe$_2$Se$_4$ (Me = Ti; V; Cr; Fe; Co; Ni) Compounds

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Abstract

Magnetization of MeFe$_2$Se$_4$ (Me = Ti; V; Cr; Fe; Co; Ni) compounds at low temperatures has been investigated. It is shown that these compounds are ferrimagnetics with low values of specific magnetization. It is established that along the crystal axis c of a given compound, there have been carried out two types of exchange interactions; cation-cation and cation-anion-cation with different dependence of their quantity on interatomic distance.

It is known that in ferri- and antiferromagnetic compounds on the basis of 3d-transition metals cation-cation as well as cation-anion-cation interactions are possible. In both cases the determinant parameter is the distance between magnetic ions. Immediate cation-cation interactions exhibit high sensitivity to change of distance between cations from the fact that interaction is proportional to the square of orbital overlap whereas interactions with the participation of intermediate anion are level considerably less dependent on distance.

In ferrimagnetic materials with spinel structures intersublattice cation-anion-cation, intrasublattice cation-cation interactions, their dependence on relative space arrangement of ions are clear.

For compounds of NiAs-type structure there is no clearity of mentioned interactions. It is connected with the complexity of their magnetic structure. So in them, instead of the usual tetrahedral interstices, there exist so-called bipiramidal interstices which are formed by means of each pair of adjacent tetrahedrons.

Relative arrangement of octahedral sublattices in these compounds differs from space arrangement of mentioned sublattices in spinel structure. So octahedrons in compounds of NiAs-type structure have common face along crystal axis c and therefore distances between magnetic ions in such octahedral interstices are comparatively small, so as to promote arising of exchange interaction along the mentioned direction.

In accordance with the considerations given above, the interrelation of magnetic and crystal structures magnetization of $MeFe_2Se_4$ (Me = Ti; V; Cr; Fe; Co; Ni) compounds crystallized in monoclinic structure of NiAs-type have been investigated in this paper.

Samples for investigation were obtained in quartz ampoules. X-ray diffraction analysis made it possible to establish the single-phase nature of the specimens and to determine the lattice parameters, as given in Table 1.

Table 1.

	$CrFe_2Se_4$	$TiFe_2Se_4$	VFe_2Se_4	Fe_3Se_4	$NiFe_2Se_4$	$CoFe_2Se_4$
a, nm	0,620	0,622	0,618	0,620	0,619	0,619
b, nm	0,354	0,354	0,352	0,353	0,354	0,353
c, nm	1,162	1,145	1,125	1,126	1,104	1,082
T_c, K	320	270	165	350	120	88

Magnetization was measured by pendulum magnetometer by Domenicalli method.

Figure 1 shows the dependence of the specific magnetization (σ) of $MeFe_2Se_4$ compounds on the magnetic field (H) at 4,2 K. Low values of specific magnetization and also character of dependence $\sigma(H)$ points to ferrimagnetic structure of these compounds. From Figure 1 it is shown that, except for Me = Cr; Ni, magnetization of all compounds reaches saturation. Magnetic insaturation of $CrFe_2Se_4$ and $NiFe_2Se_4$ appears to be connected with noncollinearity of magnetic structure.

Temperature dependence of magnetization of $MeFe_2Se_4$ compounds measured in magnetic field 12,5 koe (Figure 2) is also characteristic for materials with spontaneous magnetization.

Curie temperature (T_c) of compounds was determined by method of thermodynamic coefficients [1] and listed in Table. Obtained values of Curie temperature agree with the results of papers [2-5], devoted to investigations of thermal, elastic and electrical properties of $MeFe_2Se_4$ compounds.

As can be seen in the Table $MeFe_2Se_4$ crystal lattice parameters **a** and **b** practically do not change, with respect to parameter **c**, compounds are devided into two groups in which 3d-shell of Me is filled up by half (Me = Cr; Ti; V) and by more than half (Me = Fe; Ni; Co). In each group subsequent reduction of crystal lattice parameter **c** is observed.
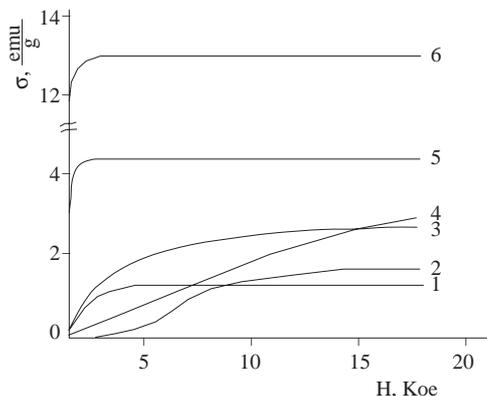
Figure 1. Depedence of the specific magnetization of $MeFe_2Se_4$ compounds on the magnetic field at 4,2K.
1. VFe_2Se_4;   2. $CrFe_2Se_4$;   3. $TiFe_2Se_4$;
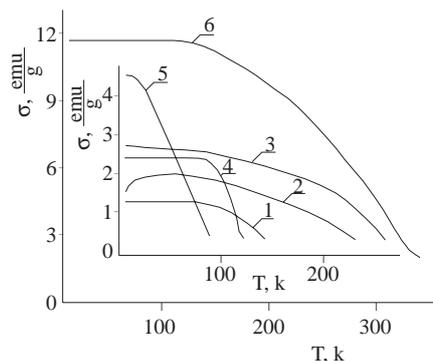4. $NiFe_2Se_4$;   5. $CoFe_2Se_4$;   6. Fe_3Se_4

Figure 2. Temperature dependence of magnetization of $MeFe_2Se_4$ compounds in magnetic field 12 koe.
1. VFe_2Se_4;   2. $CrFe_2Se_4$;   3. $TiFe_2Se_4$;
4. $NiFe_2Se_4$;   5. $CoFe_2Se_4$;   6. Fe_3Se_4

Similar decrease of Curie temperature and consequent values of exchange interaction appear to be indicative of certain bounds of exchange interaction with parameter **c**.

If it is taken into consideration that octahedral interstices of compounds with Me = Fe; Ni; Co contain Fe^{3+} ions and compounds with Me = Cr; Ti; V - Fe^{2+} ions [6] one can assume that in Fe_3Se_4, $NiFe_2Se_4$, $CoFe_2Se_4$ compounds exchange interaction is realized between Fe^{3+} ions and in $CrFe_2Se_4$, $TiFe_2Se_4$, VFe_2Se_4 compounds between Fe^{2+} ions arranged along crystal axis **c**.

However, if one assumes exchange interaction along axis **c** of one type, for example, interaction cation-cation (Fe^{2+}-Fe^{2+} or Fe^{3+}-Fe^{3+}) or cation-anion-cation (Fe^{2+}-Se^{2-}-Fe^{2+} or Fe^{3+}-Se^{2-}-Fe^{3+}) then as a result of contraction distance between Fe^{2+} (or Fe^{3+}) ions along this axis the increase of Curie temperature (i.e. exchange interaction) must be observed. Decrease of Curie temperature in a row of $CrFe_2Se_4$, $TiFe_2Se_4$, VFe_2Se_4 and Fe_3Se_4 and Fe_3Se_4, $NiFe_2Se_4$, $CoFe_2Se_4$ permits to assume simultaneous co-existence of cation-cation and cation-anion-cation interactions.

As it is shown in [7], cation-anion-cation interactions along axis **c** in compounds of NiAs-type structure are of antiferromagnetic character.

In this case, it is expected that interactions Fe^{3+}-Fe^{3+} (for Me = Fe; Ni; Co) having ferromagnetic character are weaker and they are suppressed by stronger interaction Fe^{3+}-Se^{2-}-Fe^{3+} that leads to resultant antiferromagnetic interaction. With reduction of parameter **c** and consequently with contraction of distance between cations interactions Fe^{3+}-Fe^{3+} increase stronger than interaction Fe^{3+}-Se^{2-}-Fe^{3+}. Summary interaction can remain negative and less than the initial one.

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Similar dependence of exchange interaction on parameter of crystal lattice **c** takes place for a number of $CrFe_2Se_4$, $TiFe_2Se_4$, VFe_2Se_4 compounds with the difference that in them this interaction is carried out between Fe^{2+} ions.

Thus, in $MeFe_2Se_4$ compounds, the connection between change of parameter of crystal lattice **c** and exchange interaction is established and it is shown that reduction of exchange interaction is established and it is shown that reduction of exchange interaction in a row of Fe_3Se_4, $NiFe_2Se_4$, $CoFe_2Se_4$ and $CrFe_2Se_4$, $TiFe_2Se_4$, VFe_2Se_4 is connected with the presence of two types interactions along crystal axis **c** : cation-cation and cation-anion-cation, with different dependence of their quantity on interatomic distance.

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