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The ferri-ferro-ferrimagnetic quaternary alloy

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ABSTRACT

The ferrimagnetic-ferromagnetic-ferrimagnetic quaternary alloy is constructed on the Bethe lattice in the compound form as $AB_pC_qD_r$ and formulated in terms of the exact recursion relations in the standard-random approach. The QA is designed on the BL by placing the A atoms (spin-1) only on the sites of odd shells and randomly placing B (spin-3/2), C (spin-5/2) or D (spin-2) atoms with probabilities, or concentrations, p, q and r, respectively, on the sites of even shells. The phase diagrams are obtained from the thermal analysis of the order-parameters. It is also found that the model yields only one compensation temperature.

1. Introduction

The ability of engineering and controlling the composition of many types of compound alloys should certainly serve a lot of opportunities for the improvement in science and technology. These compounds can be fabricated or found naturally in binary, ternary (TA), quaternary (QA) forms etc…with many diverse properties to be used in different areas of our daily lives. These alloys may have advantages over the other. For example, the QA magnetic semiconductor (InGaMn)As has many potential advantages which cannot be realized by TA magnetic semiconductors [1].

In the last few decades, the experimental studies of QA's have been increasing because of their possible advantages over the others. Magnetic susceptibility and Hall effect in $Pb_{1-x-y}Sn_yMn_xTe$ semi-magnetic semiconductor QA were investigated as a function of carrier concentration [2]. The magnetic properties of $R_2Re_2Si_2C$ (R = Ho and Er) were investigated by using magnetic susceptibility, magnetization and heat capacity measurements [3]. Quaternary Heusler alloy Ni_2(Mn,Fe)Ga was studied systematically for the structure, martensitic transformation, and magnetic properties in two systems [4]. The magnetic properties of the heavily Mn-doped QA ferromagnetic semiconductor $[(In_{0.44}Ga_{0.56})_{0.79}Mn_{0.21}]As$ were investigated which was grown by low-temperature molecular-beam epitaxy on InP substrates [1]. The growth of quaternary semiconductor alloy nanostructures using an example of $Zn_xCd_{1-x}S_ySe_{1-y}$ nanobelts were demonstrated for the first time [5]. The QA alkali metal, rare earth thiophosphate phase $K_4Sm_2[PS_4]_2[P_2S_6]$ was synthesized by ceramic method and characterized by using the powder X-ray diffraction, scanning electron microscope-microprobe analyses, electrochemical impedance and magnetic measurements [6]. The structural, electronic and magnetic properties in quaternary CoFeCrAl Heusler alloy were investigated [7]. The electronic and optical properties of QA GaAsBiN lattice-matched to GaAs were examined by employing first-principles combined with hybrid functional calculations [8]. The electrodeposition of QA consisting of Ni-Co-Fe-Zn was done in a chloride ion solution with the presence and absence of a Permanent Parallel Magnetic Field [9]. The single crystals of the new compound $CeCu_{0.18}Al_{0.24}Si_{1.58}$ have been grown by high-temperature solution growth method using a eutectic Al-Si mixture as flux [10]. The structural and magnetic properties of CoFeMnSi equiatomic quaternary Heusler alloy thin films were reported [11]. These references indicate that the QA's have a very wide range area of usage.

It should be noted that the theoretical studies of QA's are limited which may be caused by the complexity of these systems for theoretical handling. The existing rare theoretical studies may also be given as follows: The ordering processes in Ni-Al-Cr-X QA's (X = Co, Mo,W) were studied by using a Monte Carlo simulation technique [12]. The electronic properties, finite-temperature magnetism and transport properties of semi-Heusler quaternary alloys (Cu,Ni)MnSb were studied by means of ab initio calculations as a function of the alloy composition [13]. The band-gap design of quaternary (In,Ga)(As,Sb) semiconductors via the inverse-band-structure approach was examined [14]. The electronic and magnetic properties of the doped Heusler alloys $Co_2Cr_{1-x}V_xAl$ were studied by using first-principles density functional theory within the generalized gradient approximation scheme [15]. The first-principles calculations of the structural, electronic and magnetic properties of Heusler compounds Fe_2MnAl, Fe_2MnSi and alloy $Fe_2MnSi_{0.5}Al_{0.5}$ were presented by applying the full-potential linearized augmented plane waves plus local orbitals method based on the density functional theory [16]. Plane-wave pseudo-potential methods based on density functional theory were used to study the electronic structures, magnetic, and half-metallic properties of the equiatomic quaternary

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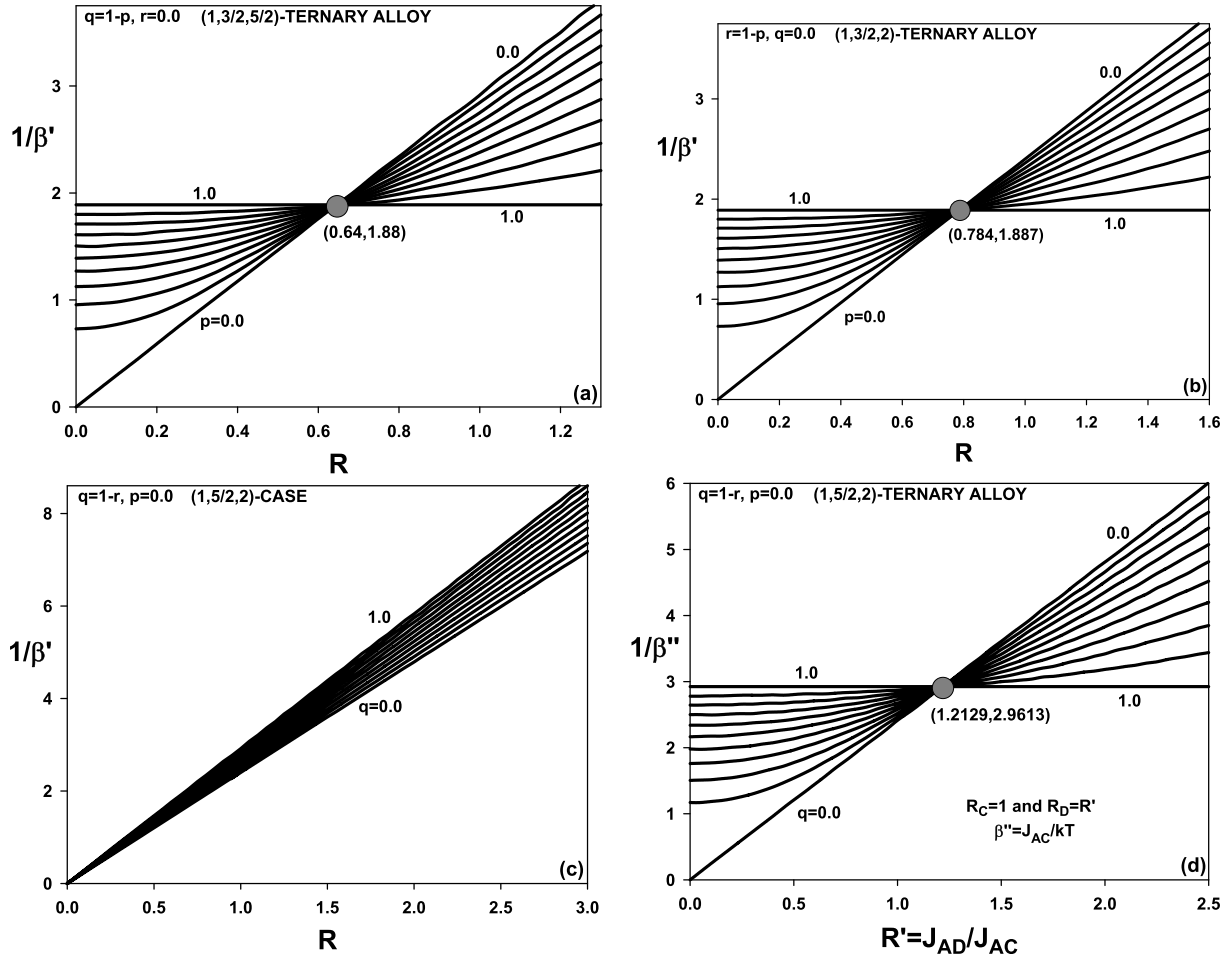

Fig. 1. The phase diagrams on the $(R, 1/\beta')$ planes with $R_C = R_D = R$; (a) (1, 3/2, 5/2)-TA model with $q = 1 - p$ and $r = 0$, (b) (1, 3/2, 2)-TA model with $r = 1 - p$ and $q = 0$ (c) $q = 1 - r$ and $p = 0$ with no corresponding TA results and (d) (1, 5/2, 2)-TA model with $q = 1 - r$, $p = 0$, $R_C = 1$, $R_D = R'$ and $\beta'' = \beta J_{AC}$.

Heusler alloys NbVMnAl and NbFeCrAl [17]. Finally, the QA consisting of atoms with spin-1/2, spin-3/2, spin-5/2 and spin-1 is simulated on the Bethe lattice (BL) with coordination number $z = 3$ corresponding to honeycomb lattice and studied in terms of exact recursion relations (ERR) in the standard-random approach [18].

In this work, we consider the QA in the compound form as $AB_pC_qD_r$ consisting of atoms of spins with spin-1, spin-3/2, spin-5/2 and spin-2, respectively, which is simulated on the BL with coordination number $z = 3$ and studied in terms of ERR's in the standard-random approach [18,19]. In this simulation, the sites of odd shells of BL are placed with the spin-1 atoms only while the sites of even shells are randomly loaded with spin-3/2, spin-5/2 or spin-2 atoms with probabilities, p, q and r, respectively. The phase diagrams are studied by the thermal analysis of the order-parameters, i.e. the magnetizations and quadrupole moments, without any distinction about the order of phase transitions because of the difficulty of their identification. The existence of compensation temperatures are also investigated and only one is found for given system parameters.

We have set up the rest of the work as follows: The formulation of the ferri-ferro-ferrimagnetic QA on the BL is given in the next section in terms of ERR's in the standard-random approach. The last section includes the phase diagrams and thermal variations of the net magnetization showing the existence of compensation temperatures in addition to the conclusions and possible comparisons.

2. The formulations in terms of ERR's

The Hamiltonian for the ferri-ferro-ferrimagnetic QA consisting of only bilinear exchange interaction parameters between the nearest-neighbor (NN) spins are given as

$$\mathcal{H} = -\sum_{<i,j>} S_i^A [J_{AB} S_j^B \xi_j + J_{AC} S_j^C \eta_j + J_{AD} S_j^D \zeta_j]. \tag{1}$$

In here, J_{AB}, J_{AC} and J_{AD} are the bilinear interaction parameters between the NN spins of $S_i^A = 1$ and $S_j^B = 3/2$, $S_j^C = 5/2$ or $S_j^D = 2$, respectively. ξ_j, η_j and ζ_j are set of random variables that can take the values of 1 or 0 depending on site j is occupied by the spin B, C or D, respectively, satisfying the normalization condition $\xi_j + \eta_j + \zeta_j = 1$. They are distributed according to

$$P(\xi_j) = p\delta(\xi_j) + q\delta(\eta_j) + r\delta(\zeta_j) \tag{2}$$

where p is the concentration of B atoms or the probability of site j being occupied by the B atoms, q is for the C atoms and r is for the D atoms similarly.

The BL is set up in such a way that the central-spin is picked to be type A with $S_i^A = \pm 1, 0$ (shell 1), to which z NN's X atoms of either type B ($S_j^B = \pm\frac{1}{2}, \pm\frac{3}{2}$) with probability p, type C ($S_j^C = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}$) with probability q or type D ($S_j^D = \pm 2, \pm 1, 0$) with probability r are added randomly forming the shell 2. Then to each X atoms on the second shell, $(z - 1)$ A atoms are added. This procedure is repeated continuously until the thermodynamic limit is reached. As a result, the odd shells of BL with $i = 1, 3, 5, \ldots$ consist of A atoms only and the even shells with $j = 2, 4, 6, \ldots$ are occupied by either B, C or D atoms with probabilities p, q and r respectively, according to Eq. (2). Thus, in this approach the even shells consist of only one type of atoms: B, C or D.

The formulation of the QA is quite simple if the ERR's for the mixed-