Onset of itinerant electron magnetism in $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys

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Onset of the magnetic order in $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys caused by Ni and Cu substitutions is studied in *ab initio* framework using density functional theory and the coherent potential approximation. It is found that Ni and Cu atoms energetically prefer Ga sites and, contrary to the earlier interpretation, the magnetism develops on the Co sublattice rather then being induced by magnetic Co antisites atoms moved to the Ga sublattice. The changes in the local electronic density of states of Co caused by Ni and Cu substitutions on Ga sublattice lead to the Stoner instability at some critical alloy composition and weak itinerant ferromagnetism, similar to that observed in $ZnZn_2$ and Ni_3Al compounds, develops.

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I. INTRODUCTION

In recent years one can note strong enhancement of experimental and theoretical interest in such traditional field of magnetic research as weak itinerant ferromagnetism (WIF). The WIF materials such as $ZrZn_2$ or Sc_3In with small magnetic moment (order of $10^{-1}\mu_B$/atom) and low Curie temperature have attracted a great deal of interest in the past since they are considered to be a limited case of itinerant (as opposite to localized) metallic magnets and thus provided a background for testing various models of itinerant electron magnetism.[1–3] The modern line of development in this field was inspired by recent experiments[4,5] with UGe_2 and $ZrZn_2$ where it has been shown that critical fluctuations existing on the border of magnetic instability of itinerant electron system may lead to very intriguing physical phenomena at low temperatures. Taking into the account a possibility to drive these metallic systems closer to the magnetic quantum critical point by applying pressure, external field or making suitably chosen chemical substitution, it appears that WIF materials are excellent candidates for study the phenomenon of quantum criticality.

Since only limited number of WIF compounds has been known, see, e.g., the overview given by Takahashi,[6] a considerable experimental effort was made in recent years to extend their list.[7–10] One of the obvious strategies is to look at the alloys of magnetic transition metals elements with nonmagnetic partners trying to identify a critical region of the compositions on the border between magnetically ordered and paramagnetic phases. In the vast majority of magnetic alloys, however, this strategy fails due to two common reasons: (1) the well-defined local atomic moments of magnetic atoms continue to exist in the paramagnetic alloys, often resulting in the appearance of an intermediate spin-glass phase or a "super" paramagnetic state. The magnetic order disappears due to reaching, e.g., the magnetic percolation threshold. (2) The crystal structure of the alloy changes or even the alloy becomes unstable, before the critical region of chemical concentrations is reached. This case occurs quite often since there are strong connections between the chemical bonding and magnetism.

A limited number of alloys where the critical region of WIF exists have attracted a special experimental and theoretical interest. The examples (see Ref. 6, and references therein) include Ni-Al, $Zr_{1-x}Ti_xZn_2$, Y_2Ni_x, and Pt-Ni systems. Another notable example is weak itinerant ferromagnetism found[11] in $Y(Co_{1-x}Al_x)_2$ where the magnetic instability of Co in paramagnetic YCo_2 is caused by the substitution of 11% of nonmagnetic Al. This intensively studied phenomena[12,13] was explained[14] as being entirely due to the effects of chemical disorder induced by Al on the electronic structure of Co. We will show here that this mechanism plays an important role also in developing of WIF state in $CoGa_{1-x}(Ni,Cu)_x$ alloys, but in contrast to the $Y(Co_{1-x}Al_x)_2$ the nonmagnetic substitutions populate in this case the nonmagnetic Ga sublattice. The general interest in studies of such phenomena may be further illustrated by mentioning two interesting, but surely more complicated for first-principles theoretical studies, problems in the physics of uranium-based intermetallics. The first one is related to the UCoAl compound which found to be strongly exchange enhanced Pauli paramagnet which exhibits[15] a first-order metamagnetic transition into WIF state in a weak applied magnetic field ($\sim$1 T). In this material the magnetism appears on U sites whereas Co is found to be nonmagnetic. An intriguing property of this compound is that the WIF ground state can be induced by making either a small amount of substitution of nonmagnetic Y or Lu in U sublattice[16] or by some nonmagnetic substitution of other T element in Co sublattice.[17] The second problem is connected to magnetic transformations in $U(Ru_{1-x}Rh_x)_2Si_2$. This celebrated material is now in focus (see, e.g., Ref. 18) of attention in the field of strongly correlated electron systems in connection with the superconductivity and quantum critical behavior found in intermediate region of Ru and Rh concentrations between of two magnetically ordered phases.

The studies of the magnetic properties of the family of $CoGa_{1-x}T_x$ (T=transition metal) alloys with ordered CsCl ($B2$) structure started in the middle of 1970's in an attempt to understand the magnetic properties of Co_2GaT Heusler-type of alloys. However, the development of magnetic order in initially paramagnetic CoGa due to substitution of T elements for Ga has attracted a special interest of many research groups due to variety of mechanisms involved in the magnetic order formation. Entire development has been reviewed

by Booth[19] (see also Stefanou *et al.*[20]). It has been widely accepted[19] that a magnetic order in $CoGa_{1-x}Co_x$ alloys is due to intrinsically magnetic Co antistructure (AS) atoms on Ga sublattice. In the range of AS Co concentrations lower than critical ($x<0.07$) an intermediate spin-glass phase in annealed samples was observed.[21] In contrast in the case of $T=V$, Ti, Mn, Fe, or Cr the ferromagnetism seems to be associated with the appearance of the magnetic moments on Co atoms on normal sites.[19] This conclusion is strongly supported by the experimental fact that in all of these alloys the ordering occurs at the same concentrations of the valence electrons.[19,22] The band structure of pure CoGa was first calculated by Whittle *et al.*[23] and than Stefanou *et al.*[20] performed calculations of magnetic state of T impurities in CoGa. Their results appear to be consistent with both discussed above scenarios of ferromagnetic order formation.

The situation with $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys, however, appears to be slightly controversial. For these alloys, in contrast to other alloys of the $CoGa_{1-x}T_x$ series, only one experimental study was reported.[24] The ferromagnetic ordering has been detected for Ni and Cu concentrations much higher than in corresponding systems with $T=$V-Fe. The authors of this study[24] have suggested that ferromagnetism appears due to Co AS atoms which moved to the Ga sublattice, whereas Ni and Cu substitutions populate Co sublattice so that the onset of the ferromagnetic order has origin similar to the $CoGa_{1-x}Co_x$ case. One of the arguments toward this scenario was the observation of superparamagnetism in the intermediate region of T concentrations. However it was also noted that the existence of the second phase in the studied samples which forms magnetic clusters of considerable size what "adding considerably to the interpretative problems" (Ref. 24) and they may be the source of strong superparamagnetic behavior. It has been also find that annealed samples have higher critical concentrations for onset of ferromagnetism than quenched ones.

In view of the interpretative complications stated above we begin our study by calculating total energies of the Ni and Cu doped alloys with different site occupations. From the results presented in the next section it appears that both Ni and Cu atoms strongly prefer Ga sites. In Sec. III we study the mechanism of magnetic instability in these alloys and have shown that at a critical Ni or Cu concentration the itinerant ferromagnetism continuously develops on Co sublattice being caused by the electronic structure effects due to Ni and Cu substitutions on Ga sublattice. It appears that $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys may be added to the list of materials for study weak itinerant ferromagnetism and critical phenomena on the border of magnetic instability.

II. METHOD OF CALCULATION AND STUDY OF CHEMICAL ORDERING

The electronic structure, total energies, and densities of states (DOS) of $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys with ordered $B2$ structure has been calculated using the *ab initio* Korringa-Kohn-Rostoker (KKR) method in the atomic sphere approximations (ASA) as described together with details of implementation in Refs. 25 and 26. Effects of exchange and correlation are treated within the framework of the local spin-density approximation (LSDA) and general gradient approximation (GGA) in Perdew-Burke-Ernzerhof parametrization.[27] The use of GGA is required, as it is usually the case for T compounds, for an accurate description of the equilibrium lattice constants of considering alloys. The effects of chemical disorder due to Ni and Cu substitutions were treated using the conventional coherent potential approximation (CPA). The convergence of the results was achieved using 7920 k points in the full Brillouin zone. The radii of ASA spheres were set to be equal for both sites of $B2$ structure and *spdf*-basis set used. The total energy calculations with fixed spin moment (FSM) constrain were done using a scheme similar to those described, e.g., by Sandratskii.[28]

The standard ASA assumes that only spherical part of the potential is used. However, in the present study the multipole corrections to electrostatic potential up to $l=3$ were used for total energy calculations as described with details of implementation by Ruban *et al.*[29] The use of these corrections makes[29] the description of configurational alloy energetic comparable to calculations with use of full charge density.

The calculations in Sec. IV are performed for GGA equilibrium lattice constants, which are calculated for every considering chemical concentration. They are presented in Fig. 1 and found to be very close to experimental[24] ones determined for annealed samples. The calculated LDA values are much lower than experimental and calculated GGA ones (not shown in Fig. 1), e.g., for $Co(Ga_{0.9}Ni_{0.1})$ LDA gives 5.245 a.u. and for $Co(Ga_{0.9}Ni_{0.1})$-5.250 a.u. The GGA values slightly decrease with increasing Ni and Cu concentrations and follow the experimentally observed trend.

As it has been shown by extensive calculations of segregation energies of binary metallic alloys (see for a review Ref. 25), the CPA-based *ab initio* scheme employed in this paper reproduces the total energy differences associated with varying site occupations in alloys of the same chemical composition very well.

III. ATOMIC DISTRIBUTION AND PARAMAGNETIC STATE

In order to find the most energetically favorable site distribution of Ni and Cu atoms we have calculated the total energies for three different site occupations in $CoGa_{0.9}T_{0.1}$ compositions: (1) Ni (or Cu) atoms are placed only on Ga sublattice, (2) Ni (or Cu) are equally distributed between Co and Ga sites, in this case part of Co moves to the AS positions, (3) All T atoms placed on the Co sublattice, and all replaced Co moves to the Ga sites. For consistency of the total energies comparison the equilibrium volume was found in all cases and respective energies are taken. It should be noted, however, that energy changes due to volume differences provides only very small corrections. The CPA provides a total energy per configuration averaged over all possible chemical configurations with given atomic site distribution. So by comparing the calculated CPA energies given in Table I we compare effectively the enthalpies of formation at $T=0$ K of alloys with the same atomic compo-

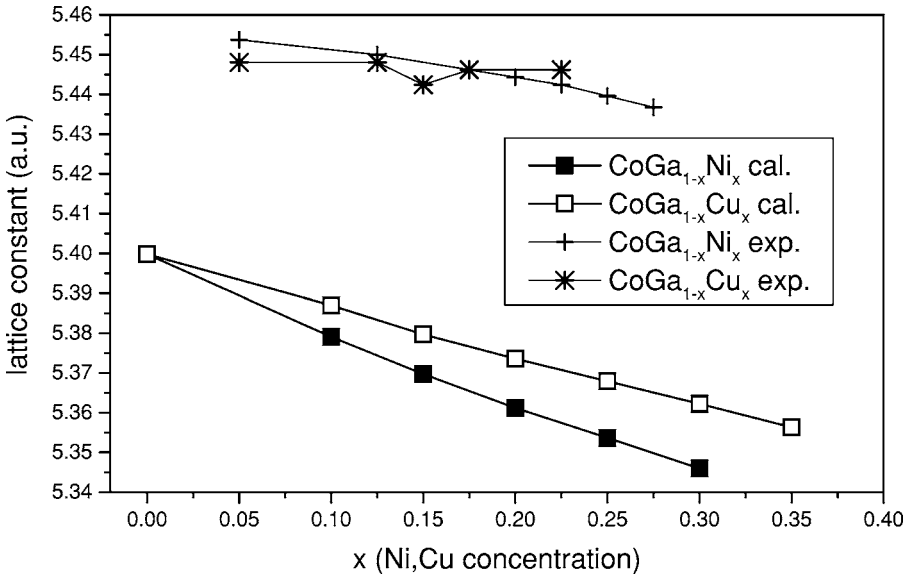

FIG. 1. Calculated (GGA) and experimental (Ref. 24) equilibrium lattice constants of $CoGa_{1-x}T_x$ alloys.

sition, but with different site occupations. These occupations are considered as macroscopic thermodynamic parameters.

The results are presented in Table I, where the energy of the most stable configuration is set to zero. It can be seen that Ni and Cu strongly prefer Ga sites. This tendency is stronger in the case of Cu which qualitatively can be well understood from the relative position of Co, Ni, Cu, and Ga in the fourth period of the Periodic Table. The results of GGA and LSDA calculations are qualitatively similar. The LSDA produces larger energy differences than GGA, but it very purely describes the equilibrium lattice constant compare to the experiment (see previous section).

An experimental study of the structural phases of $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys was performed in the late 1970's by Booth *et al.*[24] The authors argued that Ni seems to populate Co sites with displaced Co moving to the Ga sublattice. However, they also claimed that their theoretical analyzes of the results were based on the assumption of the single phase solid solution as Ni is added whereas metallographic analyses of their samples showed presence of large (~ 3 μm) precipitates, so that further more detailed study is required.[24] In case of Cu it was impossible to draw any decisive conclusion about site distribution of Cu atoms. The results of our *ab initio* study (Table I) confront these earlier conclusions. The scenario in which Ni atoms replace Co and Co atoms move to Ga sites is very energetically unfavorable. Thus, following the authors of Ref. 24 we should conclude that more refine experimental studies on good samples are necessary to resolve the issue of sites ordering in $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys. Moreover, the results presented in the next section indicate that the appearance of the magnetic order above critical concentrations of Ni and Cu is intrinsic property of most energetically stable atomic configurations namely when Ni and Cu occupy the Ga sites.

TABLE I. Calculated GGA (in brackets LSDA) total energies of $CoGa_{0.9}T_{0.1}$ (T=Ni,Cu) alloys with different site occupations. The energies are given per one T atom.

Alloy	E(mRy), T=Ni	E(mRy), T=Cu
$(Co)(Ga_{0.9}T_{0.1})$	0.00(0.00)	0.00(0.00)
$(Co_{0.95}T_{0.05})(Ga_{0.9}Co_{0.05}T_{0.05})$	7.64(14.4)	37.1(46.4)
$(Co_{0.9}T_{0.1})(Ga_{0.9}Co_{0.1})$	16.4(27.8)	70.6(88.9)

It must be noted, however, that in real samples, depending on their purity, heat treatment, or detail of the preparation, the Co atoms may appears on energetically unfavorable Ga positions. Therefore and also since in the next section we will concern only with the magnetic properties of energetically most stable (ideal) atomic configurations, we outline here the situation where Co goes on Ga sites. The calculations show that the ground state configuration from Table I, namely, $(Co)(Ga_{0.9}T_{0.1})$ is a simple Pauli paramagnet. In contrast, if Co atoms appear on the Ga site they possess an intrinsic magnetic moment. The earlier Stefanou *et al.*[20] results for single isolated Co defect atom on Ga site gives $2.09\mu_B$/atom. The calculated atomic moment on the Co AS atoms for all cases presented in Table I is almost independent on the concentration of the Co on Ga sublattice as well as on the type of T substitution being equal to $1.62\mu_B$. The case dependent deviations from this value are less than $0.02\mu_B$ and are caused mainly by differences in the equilibrium lattice constants. At the same time the Co atoms on the normal sites as well as Ni atoms on both sites stay nonmagnetic. In our calculations the small magnetic moment ($\sim 0.01\mu_B$) appears on these atoms due to band polarization originated from Co AS moments. Thus, the presence of large amount of Co AS atoms is indeed a possible reason, together with presence of the magnetic precipitates of the second phase, for superparamagnetic behavior of the samples investigated in Ref. 25. One must note, however, that magnetic ordering above critical Ni concentration would occur only if Co on the normal sites would become magnetically unstable, not by AS Co atoms alone, since (1) the concentration of magnetic Co AS in the region of considering alloys compositions is too low to create a percolation cluster, taking also into the account that replacing of the Co by Ni and consequent ap-

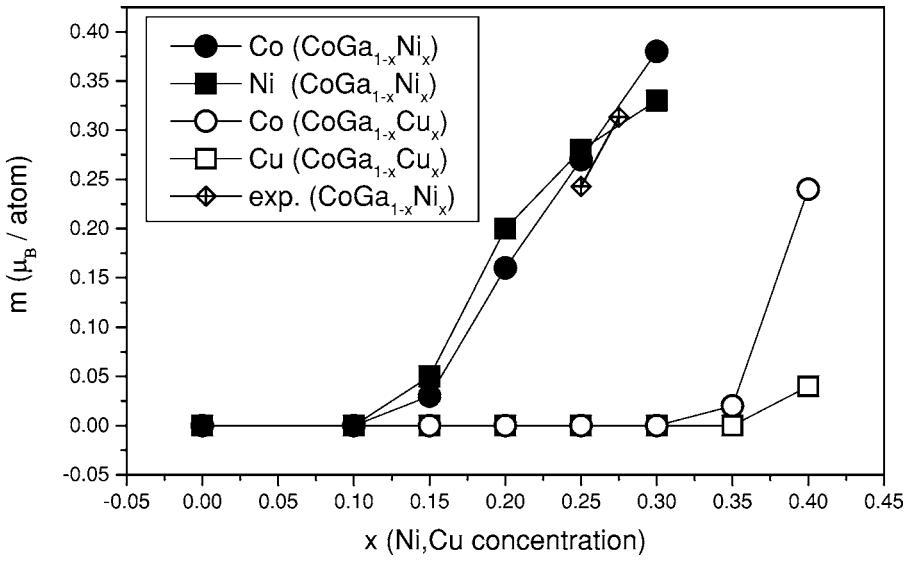

FIG. 2. Calculated ground-state magnetic moments of $CoGa_{1-x}T_x$ alloys. Experimental points were subtracted from total magnetization measurements in Ref. 24 and given in μ_B/T atom (T=Cu, Ni).

pearance of the Co AS is energetically non-favorable and (2) the fixed spin moment calculations, as well as a calculated DOS of Co on normal site presented in the next section, rule out any possibility of the itinerant electron metamagnetism scenario. The presence of some amount of Co AS may shift the actual value of the critical Ni concentration toward the lower values compare to the ideally ordered samples, but physics behind the magnetic instability of normal Co would remain unchanged. Indeed in the experiment[24] the fast quenched samples of $Co(Ga_{1-x}Ni_x)$ become ferromagnetic at $x=0.225$ whereas[30] annealed samples only at $x=0.25$. The experiment (Ref. 25) does not show a spin-glass behavior in both considering classes of alloys with Ni and Cu, whereas the $Co(Ga_{1-x}Co_x)$ alloys are spin glasses.[21] This observation indeed can serve as additional argument to the validity of our interpretation. If Co AS atoms would be responsible for magnetic order in $Co(Ga_{1-x}Ni_x)$ than one could expect that they would be spin-glasses in some region of concentrations as it is the case in $Co(Ga_{1-x}Co_x)$ alloys.

IV. ONSET OF THE MAGNETIC ORDER

The results of the calculations, presented in the previous section for $Co(Ga_{1-x}T_x)$ with $x=0.1$, have shown that lowest energy atomic configurations are those in which Ni and Cu appears only on the Ga sites. This is also the case for other alloy compositions with different T concentrations x. The ground-state configuration of $Co(Ga_{0.9}T_{0.1})$ alloys was found to be non-spin-polarized (Pauli paramagnet), whereas in the configurations where the Co atom appears on Ga sites it has a magnetic moment with value which does not depend neither on the AS concentration or type of T (Ni or Cu) substitution. Here we will show that this situation remains up to some critical concentration of the Ni or Cu impurities is reached. Than a magnetic instability on the normal Co sites develops resulting in the onset of the magnetic order. This instability is an intrinsic property of the ground-state atomic configuration without magnetic Co AS. In the following we present the results only for this ground-state atomic configurations. The calculated atomic magnetic moments are shown in Fig. 2. The critical concentration for Ni substituted alloys is $x_c \equiv 0.15$, whereas for Cu it is $x_c=0.35$. In experiment[24] the ferromagnetic order has been detected for Ni at $x=0.25$ and for Cu at $x=0.275$ (annealed samples). The source of some discrepancy may be the claimed presence of the magnetic precipitates and certain amount of Co AS atoms in the samples. At the same time one can note the good agreement between calculated and experimental atomic moments in $Co(Ga_{1-x}Ni_x)$ magnetically ordered alloys in Fig. 2.

A gradual increasing of the ground state moment in $Co(Ga_{1-x}Ni_x)$ with increasing Ni concentration from zero value to couple of tenth μ_B over wide range of concentrations is clearly seen. In the concentration range from $x=0.15$ to $x=0.25$ the ideal $Co(Ga_{1-x}Ni_x)$ samples should be weak itinerant ferromagnets with very small moment. It is also interesting to see that magnetic moments appear simultaneously on both Co and Ni sites signaling a very itinerant character of the magnetism in the broad vicinity of the critical concentration. In Cu substituted alloys the magnetic moment of Cu is much smaller than those of Co and merely the effects of the band polarization induce it.

The stability of the calculations was checked using the fixed spin moment (FSM) approach, where the total energy of $Co(Ga_{1-x}Ni_x)$ has been calculated by fixing the total moment of the unit cell. The results of these calculations are presented in Fig. 3 and they vividly illustrate the gradual development of the WIF states. The minimum of the total energy versus moment curve does not develop until the first derivative at $M=0$ becomes negative (Stoner criterion). So that a possibility of metamagnetic like transition, in which some high moment state becomes abruptly stable at some Ni concentration, should be ruled out. This means that the onset of the magnetism in these alloys may be indeed regarded as a sort of quantum phase transition where the role of the external parameter is played by the concentration of Ni atoms. Although such kind of criticality is not always accepted by some authors as a "true" quantum critical point, in any case strong itinerant spin fluctuations are expected to be present in the considering alloys in the vicinity of the critical concen-

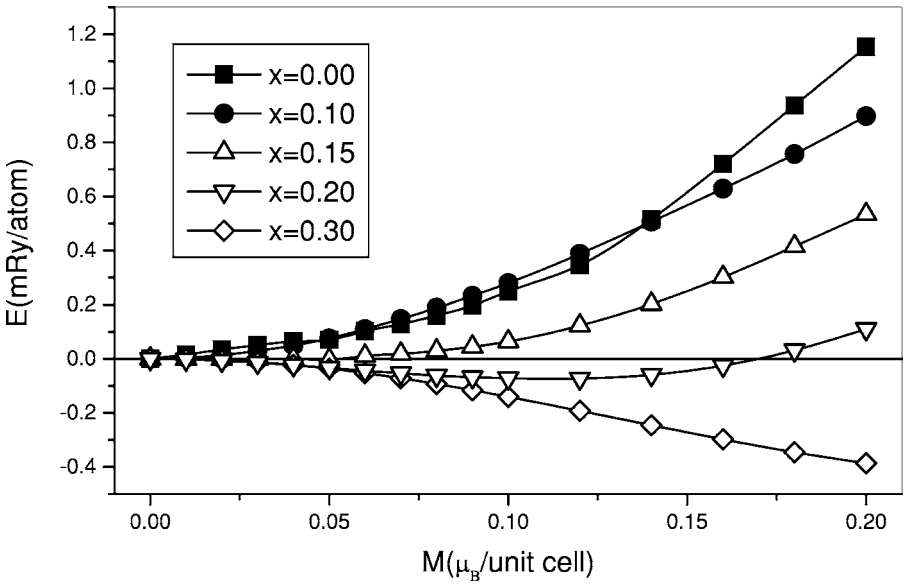

FIG. 3. FSM total energies for $CoGa_{1-x}Ni_x$ alloys.

tration. It must be noted that an existence of strong charge fluctuations, which may not be taken into account properly in the LSDA based scheme, may eventually suppress the second order quantum phase transition, as it has been shown in the framework of one-band Hubbard model in Refs. 31 and 32. However, an assessment of this interesting scenario in the LSDA first-principles framework is hardly possible at present.

In $Co(Ga_{1-x}Cu_x)$ alloys the magnetic moments develop on the Co sublattice, whereas Cu has only induced moment. In contrast in $Co(Ga_{1-x}Ni_x)$ above x_c both Co and Ni become magnetic simultaneously. However, their role in the establishment of overall magnetic order is not equivalent. In order to investigate this issue in detail we have performed additional set of FSM calculations in which the magnetic moment was fixed separately on Co and Ni sites in otherwise magnetic $Co(Ga_{0.8}Ni_{0.2})$. The calculations in which the Ni moments were fixed to zero and Co moments remain unconstrained lead to the magnetic self-consistent solution with finite Co moment as it happens also in the fully unconstrained calculation. In contrast, in the calculations where the Co moments was set zero and Ni moments were relaxed the Ni moment vanished. Thus, it can be concluded that also in Ni substituted alloys the magnetism appears entirely due to the magnetic instability of the Co sublattice.

V. CONCLUSIONS

In this paper we have shown that itinerant ferromagnetism continuously develops on Co sublattice of $Co(Ga_{1-x}Ni_x)$ and $Co(Ga_{1-x}Cu_x)$ alloys at some critical alloy composition. The study of magnetism in this class of alloys, reported[24] almost 30 years ago, has certainly not exploited all of their eventually interesting properties revealed in this work. The possibility of occurence of the weak itinerant ferromagnetism on the Co sublattice due to doping Ga sites with nonmagnetic substitutions may be very interesting in the context of the modern studies of itinerant magnets on the border of magnetic instability.

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