



Effect of thermal expansion, electronic excitations, and disorder on the Curie temperature of $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys

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We demonstrate the importance of thermal effects such as temperature-induced electronic, magnetic and vibrational excitations, as well as structural defects in the first-principles calculations of the magnetic critical temperature of complex alloys using half-Heusler $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys as a case study. The thermal lattice expansion and one-electron excitations have been accounted for self-consistently in the Curie temperature calculations. In the Ni-rich region, electronic excitations, thermal expansion, and structural defects substantially decrease the calculated Curie temperature. At the same time, some defects are shown to increase T_C in Cu-rich samples.

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I. INTRODUCTION

The magnetic critical temperature, the Curie temperature (T_C) in ferromagnets and the Néel temperature (T_N) in antiferromagnets, is among the most important parameters of magnetic materials, which determines in many cases the upper limit of the operational temperature range of magnetic devices. It is therefore desirable both to understand the mechanisms governing the critical temperature and to be able to predict it from first-principles calculations. However, in spite of a substantial progress in the first-principles-based methods, accurate and reliable theoretical predictions of the magnetic transition temperature are still a great challenge due to the extreme complexity of the problem. For quantitative predictions, both finite-temperature magnetic excitations as well as the influence of structural, chemical, thermal and other effects on the magnetic interactions must be accurately accounted for.

The widely used procedure in such calculations consists of a mapping of the configurational magnetic energetics of local atomic moments onto a Heisenberg or related Hamiltonian using, for instance, the magnetic force-theorem method.¹ The critical temperature can then be obtained in subsequent statistical-mechanics simulations. In spite of the fact that such calculations are based on many idealizing assumptions and rather strong approximations, unavoidable at present due to complexity of the problem, they occasionally show excellent agreement with experimental data. This is frequently used for claiming the validity of the whole theoretical framework. Vice versa, if a straightforward approach does not reproduce expected results, it is accustomed to refer to inaccuracies on the most fundamental level of the theory, blaming for instance, an approximate description of exchange-correlation interactions. This is done without a sufficient consideration of other effects, such as structural disorder and different kinds of thermal excitations, in spite of the fact that the latter is inevitably present in real systems under given experimental conditions close to the transition temperature.

Indeed, there are many sources of error in the usual first-principles approach. First of all, the discrepancies between

theory and experiment originate from the fact that the chosen magnetic Hamiltonian cannot in practice include all the possible dependencies of the magnetic interactions on the external and internal conditions. Second, the details of exchange interaction parameter calculations can greatly affect the results, which of course also include inaccuracies of the exchange-correlation description in the local approximation of density-functional theory. These issues are worth considering, but a close examination of the underlying physical problem gives rise to other issues, most often completely neglected, especially in the case of alloys.

First of all, the underlying atomic configurational state is usually significantly simplified, neglecting different types of structural defects or specific atomic distribution of alloy components on the lattice. Second, the reference magnetic state in the calculations of magnetic exchange interactions is frequently different from the paramagnetic state relevant at the point of the magnetic phase transition, although a very wide range of the systems exhibit a significant dependence of the magnetic exchange interaction parameters of the Heisenberg Hamiltonian on the global magnetic state.² Finally, different types of thermal excitations are neglected, since the first-principles calculations are usually done for the ground-state structure at 0 K. The latter can, in fact, be quite a severe approximation for the important class of high- T_C materials. It is clear that the accurate description of the magnetic phase transition requires consideration of the electronic structure of the system such that it presents itself around the critical temperature.

In this work, we show the importance of considering both structural and magnetic disorder, thermal excitations, such as thermal lattice expansion and one-electron excitations in the calculations of the magnetic critical temperature of half-Heusler $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys. This system has recently attracted considerable attention³⁻⁵ because of its relevance to spintronics⁶ and an unusual transition from high- T_C ferromagnetism in NiMnSb to antiferromagnetism in CuMnSb . From the theoretical point of view, this system also presents a certain puzzle, since all the existing first-principles-based calculations yield too high value for the Curie temperature of

NiMnSb (838–1210 K),^{7–10} compared to the experimental one (718–756 K).^{11–17}

II. CALCULATIONAL METHODS

The starting point in our calculations of T_C for $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys is the Heisenberg magnetic Hamiltonian

$$H = - \sum_{i \neq j} J_{ij} \mathbf{e}_i \cdot \mathbf{e}_j, \quad (1)$$

where \mathbf{e}_i is a unit vector in the direction of the local magnetic moment at site i , which is applied only to Mn atoms. That is, already at this stage we neglect (1) the dependence of magnetic exchange interaction parameters on the underlying magnetic state, (2) the possible contribution from longitudinal spin fluctuations and as a result, and (3) the magnetic interactions between Ni and Mn atoms in the paramagnetic state. As shown by, for instance, Sasioglu *et al.*,⁷ the magnetic exchange interaction in NiMnSb indeed depends on the magnetic state, so the system cannot be strictly considered as a Heisenberg ferromagnet. However, we assume that the magnetic exchange interactions in the paramagnetic state do not show their dependence on particular local orientations of magnetic moments on Mn atoms, and we primarily use the paramagnetic state as a reference state in the calculations of the magnetic exchange interactions. For comparison, we also derive exchange interaction parameters in the ferromagnetic (FM) state, ignoring Mn-Ni interactions as envisaged in Ref. 5.

A mean-field approach based on the method presented in Ref. 18 has been used in order to estimate the effect of temperature-induced longitudinal spin fluctuations at 800 K in NiMnSb. Although the local magnetic moment on Mn atoms are practically unaffected, the average magnitude of local magnetic moments on Ni atoms at this temperature in the paramagnetic state is about $0.37\mu_B$. This actually means that this is not a Heisenberg system at high temperature, and in accurate theoretical consideration the temperature-induced longitudinal spin fluctuations should be taken into account. Nevertheless, we ignore them in this study mostly due to the complexity of the problem, although we believe that their contribution to the transition temperature is relatively small in line with previous investigations of the Ni-Mn interaction in NiMnSb.^{9,10} Besides, our objective is to demonstrate the importance of other effects. Let us note that longitudinal spin fluctuations on Ni atoms were already considered by Lezaic *et al.*⁸ and Sandratskii,¹⁹ who focused on low-temperature magnetic properties.

The disordered local-moment (DLM) (Ref. 20) model has been employed for the description of the paramagnetic state. Within this model, Mn atoms with spin-up and spin-down orientations of magnetic moment constitute a random alloy on the corresponding sublattice. The magnetic exchange interactions have been calculated using the magnetic force-theorem method¹ in the paramagnetic (J_{ij}^{DLM}) and ferromagnetic (J_{ij}^{FM}) states. The electronic structure calculations have been done by the exact muffin-tin orbitals (EMTOs) (Refs. 21 and 22) method using the generalized gradient approxi-

mation (GGA) (Ref. 23) for the exchange-correlation energy. The coherent-potential approximation (CPA) (Ref. 24) has been used to account for a random distribution of atoms, in the disordered local-moment model, as well as for structural defects. The full charge-density technique²⁵ has been used in the total-energy EMTO calculations.

In order to take the thermal lattice expansion and electronic excitations into account, T_C (T_N for CuMnSb) have been calculated by using the following self-consistent scheme. (1) First, the initial magnetic interaction parameters were obtained at 0 K for the corresponding lattice spacing. (2) A Heisenberg Monte Carlo technique was used in order to calculate T_C . (3) A updated set of exchange interaction parameters was obtained for the lattice parameter corresponding to the transition temperature T_C determined in the previous step. The thermal lattice expansion has been determined using the Debye-Grüneisen model.²⁶ Thermal one-electron excitations corresponding to the same temperature were also taken into account. (4) T_C was recalculated with the updated set of interactions by the Monte Carlo method. Steps (3) and (4) were then repeated until T_C was converged. In all cases considered in this study, T_C was converged within the accuracy of the Monte Carlo simulations after four iterations.

Magnetic interaction parameters as well as thermal expansion have been determined independently for each concentration of Ni and Cu both for an ideal C1_b system and in systems containing different defects. A Heisenberg Monte Carlo simulation scheme capable of handling arbitrary levels of chemical disorder on the sublattices has been used to determine the Curie temperature within 15 K error bar due to the included range of interactions as well as other simulation parameters. Since the local magnetic moment on Mn defects in the interstitial and substitutional positions on the (Ni,Cu) sublattice did not disappear in the DLM state, the Mn defects were considered on equal footing with the Mn atoms on the Mn sublattice in the Heisenberg Monte Carlo simulations.

III. RESULTS AND DISCUSSION

A. NiMnSb

We first study the effects of thermal lattice expansion, Fermi-surface smearing due to thermal one-electron excitations, and the choice of magnetic reference state on T_C of pure NiMnSb. The left panel of Fig. 1 shows the lattice spacing of NiMnSb as a function of temperature calculated in the ferromagnetic and DLM states. Note that the calculated values include the zero-point vibrational energy.²⁶ The experimental points at 4 K (Ref. 14) and room temperature¹⁶ are also included for comparison. The calculated equilibrium lattice parameter at 0 K for the ferromagnetic state neglecting zero-point vibrations, the value normally referred to as “calculated lattice parameter,” is 5.95 Å. This is in good agreement with the experimental value 5.91 Å (at 4 K), showing a usual GGA overestimation of 0.6%. The lattice parameter in the DLM state, of relevance for comparison around T_C , is slightly larger at all temperatures. This observation is in line with the experimental finding that the magnetic contribution to thermal expansion is positive and shows a sharp peak at T_C .²⁷

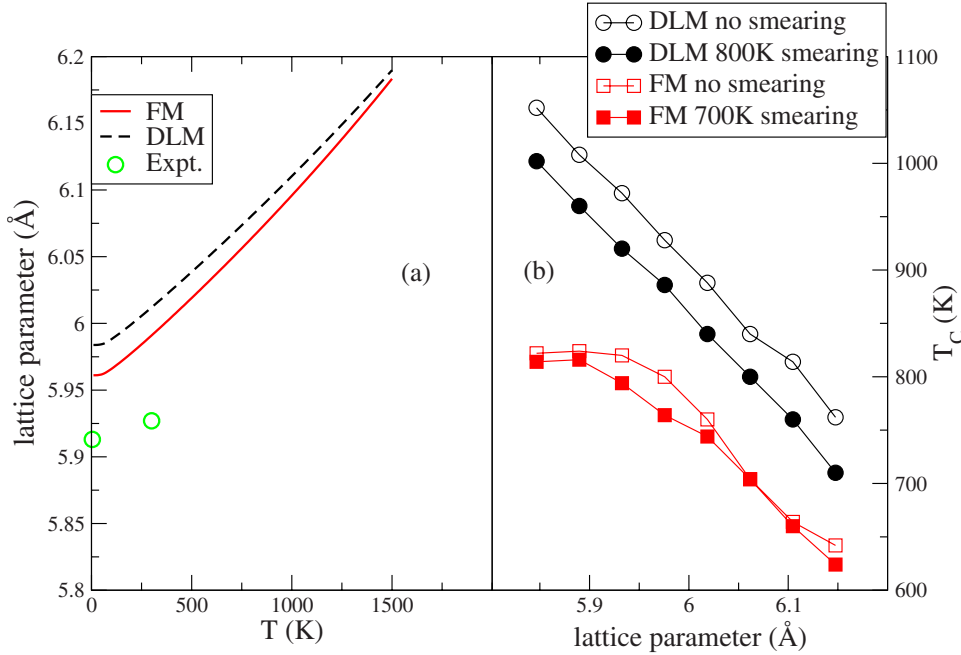


FIG. 1. (Color online) (a) Equilibrium lattice spacing of NiMnSb as a function of temperature, calculated within the Debye-Grüneisen model for the ferromagnetic (solid line), and disordered local moment (dashed line) states. The experimental values at 4 K (Ref. 14) and room temperature (Ref. 16) are shown with circles for comparison. (b) Calculated Curie temperature of NiMnSb as a function of lattice parameter using J_{ij}^{FM} (squares) and J_{ij}^{DLM} (circles) exchange interactions. Closed (open) symbols show calculations with (without) thermal one-electron excitations smearing corresponding to $T \approx T_C$.

Let us note that the thermal expansion is quite sensitive to the details of the total-energy calculations. In the present GGA calculations, the linear thermal expansion coefficient, α , is found to be $22.5 \times 10^{-6} \text{ K}^{-1}$ at room temperature for the FM state and slightly lower, $21.4 \times 10^{-6} \text{ K}^{-1}$, for the DLM state. This is an overestimation of the experimental value $15 \times 10^{-6} \text{ K}^{-1}$.²⁷ The deviation is likely to be the result of the underestimation of the bulk modulus in the GGA. Local spin density approximation (LDA) calculations produce a lower value of $15.8 \times 10^{-6} \text{ K}^{-1}$, in agreement with both the previous LDA calculations²⁸ and experiment. The LDA, on the other hand, substantially underestimates the lattice spacing of these systems, making itself nonuseful for the present study. For consistency reasons we therefore use the GGA in all calculations, keeping in mind that in reality, the effect of thermal expansion might be approximately 75% of the calculated value.

In panel (b) of Fig. 1 we show the calculated Curie temperature of NiMnSb as a function of the lattice spacing using both J_{ij}^{FM} and J_{ij}^{DLM} with and without thermal one-electron excitations at temperatures close to the self-consistent values of T_C , 700 K for the FM reference state, and 800 K for the DLM reference state. It is clearly seen that the Curie temperature is very sensitive to the lattice constant, especially in the DLM calculations; the T_C drops by 100 K with the increase in the lattice spacing from 5.97 Å (0 K DLM value) to 6.08 Å, which is the self-consistent theoretical lattice constant at T_C . The inclusion of thermal one-electron excitations lowers the Curie temperature further by 50 K bringing it to about 780 K.

The calculations using J_{ij}^{FM} yield critical temperatures considerably below the values obtained with J_{ij}^{DLM} . The J_{ij}^{FM} exchange interactions are also less sensitive to the change in the lattice spacing and thermal one-electron excitations compared to J_{ij}^{DLM} . However, there is still a decrease in T_C from 780 to 710 K when both effects are taken self-consistently into consideration. It is clear that thermal expansion in com-

ination with thermal one-electron excitations can explain at least a part of the overestimation of T_C for NiMnSb in previous calculations. Let us note that all the results presented in Fig. 1 have been obtained in the GGA. However, we have also done some test calculations within the LDA which resulted in very similar temperatures. For fixed lattice spacings the T_C calculated using the LDA exchange interaction parameters was up to 50 K higher than the corresponding GGA value.

B. Ni_{1-x}Cu_xMnSb alloys

We now turn to Ni_{1-x}Cu_xMnSb alloys. There exist two independent sets of experiments measuring T_C for $x \leq 0.90$,^{3,12} and they are both shown in Fig. 2. According to the experimental data, T_C decreases with increasing Cu content. T_C variation with composition is not linear but shows a negative curvature with faster decrease in the Cu-rich region. As one can see in Fig. 2, the Curie temperature calculated using J_{ij}^{DLM} interactions shows concentration dependence qualitatively similar to experiments. The importance of the thermal correction can be readily seen as it removes a considerable overestimation of T_C for the Ni-rich region and brings the calculated values into much better agreement with the experiments.

In alloys with higher Cu concentration thermal correction becomes less important. Partly this can be explained by the lower values of T_C , but a coupling between the valence electron concentration and the effect of thermal expansion on T_C seems to be present. The calculations using the J_{ij}^{FM} exchange interactions yield lower T_C compared to when J_{ij}^{DLM} are used. When the thermal corrections are taken into consideration, the Curie temperature becomes also lower than the experimental values for all concentrations of Cu up to $x < 0.90$. Although the FM-based calculations appear to reproduce experimental values well for $x \leq 0.20$, for higher Cu content they predict a qualitatively wrong concentration dependence,

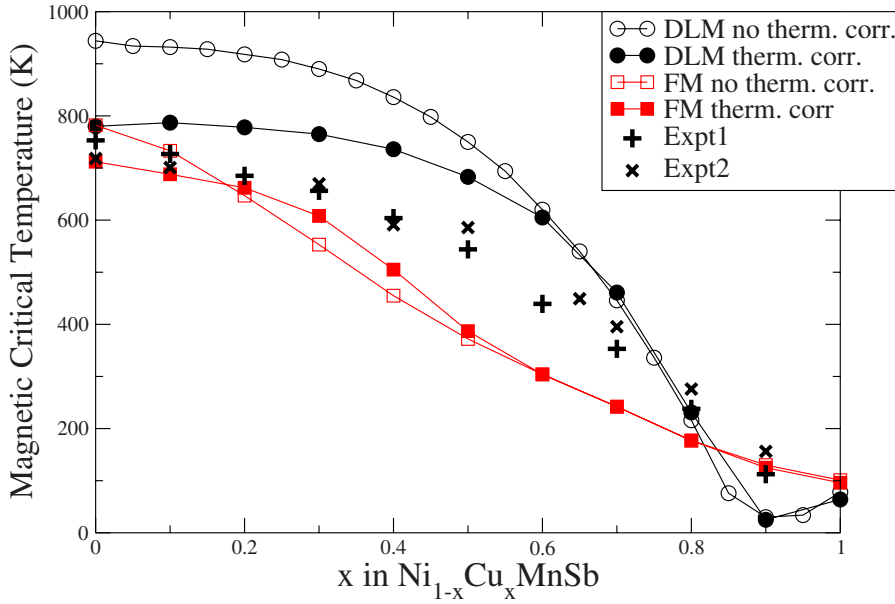


FIG. 2. (Color online) Calculated magnetic critical temperature of $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys with (solid symbols) and without (open symbols) thermal correction. Calculations using interactions derived from a paramagnetic DLM reference state are shown with circles. Calculations using interactions derived from a ferromagnetic reference state are shown with squares. Experimental series are marked with $+$ ³ and \times ¹².

showing a positive curvature of the T_C curve. This behavior was noted also in Ref. 5 and the need to account for the effect of strong electron correlations within the LDA+ U approximation was suggested. We conclude instead that it is the unjustified use of the J_{ij}^{FM} exchange interactions that leads to this behavior, since the calculations using J_{ij}^{DLM} interactions derived with the same GGA approximation for exchange-correlation effects resolve the qualitative disagreement between theory and experiments.

C. Structural defects in $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys

Let us note that the critical temperature calculated with the J_{ij}^{DLM} exchange interactions exhibits a minimum for alloy compositions around $x=0.90$. This is not surprising considering the predicted switching of the magnetic order from ferromagnetic to antiferromagnetic close to this alloy composition. At the same time, this is not what is observed experimentally; paramagnetic-to-ferromagnetic phase transitions at temperatures of 110 and 155 K are reported. A possible origin of this discrepancy is an idealized description of the atomic configuration of the $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys in the theoretical consideration, where all the possible interstitial or substitutional defects have been disregarded and an ideally random $\text{Ni}_{1-x}\text{Cu}_x$ alloy has been assumed to be present exclusively at the (Ni,Cu) sublattice.

At the same time, the experimental data indicate the existence of different types of defects in this alloy. For instance, an excess of Mn is deliberately used or observed in samples in several experiments^{16,29} and it was shown³⁰ that Mn interstitials are the most likely candidates to explain higher-than-expected results of magnetic-moment measurements for NiMnSb.^{14,31,32} Besides, several experiments have shown lower magnetic moments indicating other types of disorder. $\text{Ni}_{\text{Mn}}+\text{Mn}_{\text{Ni}}$ swap defects and $\text{Ni}_{\text{I}}+\text{V}_{\text{Ni}}$ vacancies and interstitials have been found to be two of the least energetically costly stoichiometric defects in NiMnSb.³⁰ In related PtMnSb thin films a level of 10% intersite disorder has

been observed.³³ The spread of experimental values of T_C for NiMnSb [718 K (Ref. 12)–756 K (Ref. 17)] is in itself an indication of nonideal samples. Finally, an order-disorder transition has been reported in pure CuMnSb at 753 K.¹⁶

In principle, the equilibrium amount of defects can be calculated from first-principles and included in the self-consistent scheme above. However, in many systems such as thin films and quenched bulk samples, equilibrium is not achieved and considerable levels of defects can be expected. Therefore in order to investigate the qualitative effect of the structural disorder on the critical temperature, we have considered three different cases: 5% of off-stoichiometric Mn interstitials, stoichiometric swap defects with 5% of the Mn atoms exchanging places with Ni and Cu atoms, keeping the Cu:Ni ratio on both sublattices, and finally a stoichiometric disorder where 5% of the Cu and Ni atoms are present on the interstitial position, leaving 5% of vacancies. The calculations have been performed with thermal effects included and using the independently derived J_{ij}^{DLM} exchange interactions. The results are presented in Fig. 3, and separately in Table I, we summarize our results for NiMnSb.

One can see that all three types of defects decrease T_C in the Ni-rich alloys, bringing theoretical results into even better agreement with the experimental data. While Mn intersti-

TABLE I. Thermally corrected, T_C^c , and uncorrected, T_C^u , calculated values of the magnetic critical temperature in K using a DLM reference state for ideal and nonideal NiMnSb.

NiMnSb	T_C^c (K)	T_C^u (K)	Expt. (K)
Ideal C1_b -NiMnSb	780	942	718–756 ^a
5% Mn_{I}	745	845	
5% $\text{Ni}_{\text{Mn}}+\text{Mn}_{\text{Ni}}$	715	815	
5% $\text{Ni}_{\text{I}}+\text{V}_{\text{Ni}}$	730	830	

^aReferences 11–17. In general, the exact site occupancies in the experimental samples are not specified or known.

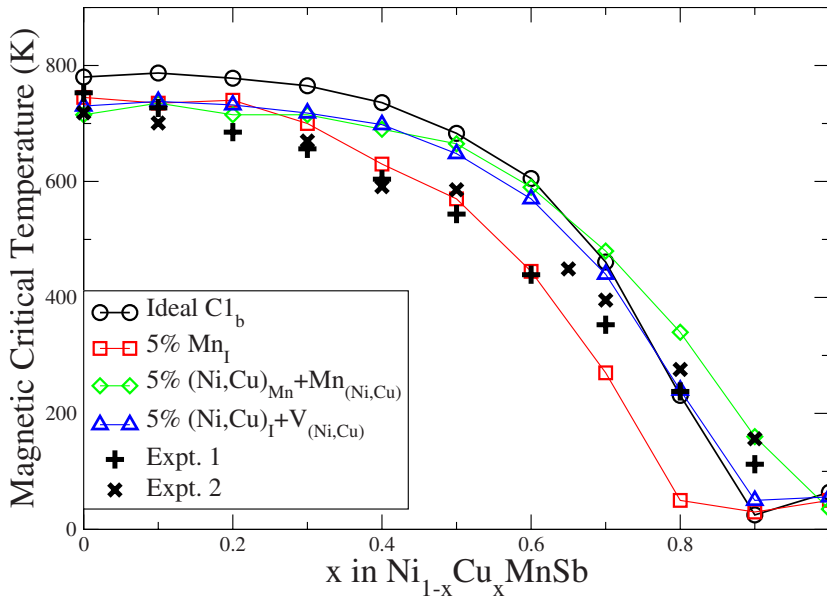


FIG. 3. (Color online) Calculated magnetic critical temperature of $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys both for ideal C1_b structure (circles), 5% Mn interstitials (squares), 5% $(\text{Ni,Cu})_{\text{Mn}} + \text{Mn}_{(\text{Ni,Cu})}$ swap defects (diamonds), (d) 5% $(\text{Ni,Cu})_I + \text{V}_{(\text{Ni,Cu})}$ interstitials + vacancies (triangles). Experimental series are marked with $+^3$ and \times^{12} .

tials decrease T_C with respect to the ideal case for almost the whole concentration range, the effect of $(\text{Ni,Cu})_I + \text{V}_{(\text{Ni,Cu})}$ defects is very small for $x \geq 0.6$. One can also see that 5% $(\text{Ni,Cu})_{\text{Mn}} + \text{Mn}_{(\text{Ni,Cu})}$ swap defects considerably stabilize the ferromagnetic state, or actually a ferrimagnetic state with the moments of $\text{Mn}_{(\text{Ni,Cu})}$ defect atoms tending to be antiparallel to the main ferromagnetic Mn sublattice, in Cu-rich alloys. This offers a possible explanation of the discrepancy between experimental data and theoretical calculations for ideal samples at $x=0.90$. In fact, our results suggest that there is a transition from a tendency to form Mn interstitials in the Ni-rich alloy toward a tendency to form $\text{Mn}_{\text{Cu}} + \text{Cu}_{\text{Mn}}$ swap defects in the Cu-rich alloys.

A test was made of the effect of 5% $\text{Ni}_I + \text{V}_{\text{Ni}}$ when T_C of NiMnSb is calculated from J_{ij}^{FM} exchange interactions. As a result of the defects T_C decreased by 57 K to 655 K in this case.

IV. CONCLUSIONS

In conclusion, we have demonstrated the importance of considering both structural defects and finite-temperature excitations when the Curie temperatures in $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ half-Heusler alloys are calculated from first principles. Taken into account altogether, those effects considerably improve the agreement between first-principles simulations and ex-

perimental studies over the whole concentration range of Cu in $\text{Ni}_{1-x}\text{Cu}_x\text{MnSb}$ alloys.

This case study also illustrates the danger of choosing theoretical methodology on the basis of agreement or disagreement with experiments, such as the nonintuitive use of the ferromagnetic rather than paramagnetic reference state advocated in Ref. 5. When further important effects are included, or when the method is applied to a larger group of systems, the initial judgment about the agreement with the experiments might be reversed. This work strongly supports the rather obvious view point that the theoretical simulations of experimentally observed properties should be done for the corresponding internal and external conditions. This implies that a disordered rather than an ordered magnetic reference state should be used to derive magnetic exchange interactions when the critical temperature is studied. We suggest that our results are general and of high importance for other magnetic alloy systems exhibiting high T_C and possible intersite disorder.

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