Martensitic transition, ferrimagnetism and Fermi surface nesting in Mn$_2$NiGa

S. R. Barman, S. Banik, A. K. Shukla, C. Kamal and Aparna Chakrabarti

1 UGC-DAE Consortium for Scientific Research - Indore, 452017, Madhya Pradesh, India
2 Raja Ramanna Centre for Advanced Technology - Indore, 452013, Madhya Pradesh, India

received 7 August 2007; accepted in final form 5 October 2007
published online 31 October 2007

PACS 71.20.Be – Transition metals and alloys
PACS 71.18.+y – Fermi surface: calculations and measurements; effective mass, g factor
PACS 81.30.Kf – Martensitic transformations

Abstract – The electronic structure of Mn$_2$NiGa has been studied using density functional theory and photoemission spectroscopy. The lower-temperature tetragonal martensitic phase with $c/a = 1.25$ is more stable compared to the higher-temperature austenitic phase. Mn$_2$NiGa is ferrimagnetic in both phases. The calculated valence band spectrum, the optimized lattice constants and the magnetic moments are in good agreement with experiment. The majority-spin Fermi surface (FS) expands in the martensitic phase, while the minority-spin FS shrinks. FS nesting indicates occurrence of phonon softening and modulation in the martensitic phase.

Introduction. – The recent advent of multiferroic-shape memory alloys (SMA) like Ni-Co-Mn-In, Ni-Mn-Ga that exhibit both ferroelastic and ferromagnetic properties has ushered a flurry of activity in this field [1–9]. In particular, Ni-Mn-Ga has generated immense interest because of very large strain (10%) in a moderate magnetic field ($\approx 1$ tesla) [3,4]. Moreover, in Ni-Mn-Ga the actuation is much faster ($\approx 2$kHz) than in conventional SMA [5]. However, Ni$_2$MnGa are brittle and so search for materials with better mechanical properties exhibiting similar magnetic-field-induced strain is being actively pursued [10,11]. Mn$_2$NiGa is a recently discovered ferromagnetic SMA in the Ni-Mn-Ga family. It has Curie and martensitic start temperatures of 588 and 270K, respectively [11]. Ferromagnetism in Mn$_2$NiGa is surprising because direct Mn-Mn interaction normally leads to antiferromagnetic alignment [12,13]. Moreover, the origin of the martensitic transition involving a relatively large tetragonal distortion ($c/a = 1.21$) has not been studied theoretically till date. Recently, a density functional theory (DFT) study on Mn$_2$NiGa shows a large enhancement of the density of states (DOS) near the Fermi level ($E_F$) and quenching of Mn and Ni magnetic moments in the martensitic phase [14]. However, such large change in the magnetic moments or DOS has not been observed in any other SMA either from experiment [9,15,16] or theory [8,17,18].

The geometry of the Fermi surface (FS) is responsible for a variety of phenomena like spin or charge density waves, Kohn anomalies, Friedel oscillations in metals. If the FS has parallel planes, strong electronic response can occur at the wave vector that translates one parallel plane of the FS to the other. This wave vector is called the nesting vector (n.v.). FS nesting has been reported to cause softening of the transverse-acoustic (TA$_2$) phonon mode along the [110] direction resulting in a modulated pre-martensitic phase of SMAs like Ni$_2$MnGa and Ni-Ti [19]. Recently, an inelastic neutron scattering study on Ni$_2$MnGa showed the presence of charge density wave in the martensitic phase resulting from FS nesting [7]. Thus, it is worthwhile to study the FS of Mn$_2$NiGa, particularly because the relatively large tetragonal distortion is likely to modify the FS substantially.

In this work, a DFT study of the electronic structure of Mn$_2$NiGa using the full potential linearized augmented plane wave method (FPPLAPW) is presented. The valence band (VB) spectrum, calculated from the theoretical DOS, is in agreement with the ultraviolet photoemission spectroscopy (UPS). We find that the total energy ($E_{tot}$) is lower in the martensitic phase with a tetragonal distortion of $c/a = 1.25$. We show that Mn$_2$NiGa is an itinerant ferrimagnet in both the martensitic and austenitic phases. The equilibrium lattice constants and the magnetic moments are in agreement with X-ray...
Diffraction and magnetization data, respectively. The FS in the martensitic phase is drastically different from the austenitic phase. A highly nested hole-type majority-spin cuboidal FS sheet around the Γ-point appears in the austenitic phase. A high-nested hole-type majority-spin in the martensitic phase is drastically different from the austenitic phase. The FS has been indexed by a tetragonal unit cell with $c/a = 1.21$ (fig. 1b) [11,16].

**Methodology.** – First-principles DFT calculations were performed using the WIEN97 code [20]. The generalized gradient approximation (GGA) for the exchange correlation that accounts for the density gradients was used [21]. An energy cut-off for the plane-wave expansion of 16 Ry is used ($R_{MTK_{max}} = 9$). The cut-off for charge density is $G_{max} = 14$. The maximum $l (l_{max})$ for the radial expansion is 10, and for the non-spherical part: $l_{max, ns} = 6$.

The muffin-tin radii are Ni: 2.1364, Mn: 2.2799, and Ga: 2.1364 a.u. The number of $k$ points for self-consistent field cycles in the irreducible Brillouin zone is 256 and 484 in the austenitic and martensitic phase, respectively.

The convergence criterion for $E_{tot}$ is 0.1 mRy, which implies that the accuracy of $E_{tot}$ is ±0.34 meV/atom. The charge convergence is set to 0.001. FS has been calculated using XcrySDen [22]. The Mn$_2$NiGa ingot was prepared by arc furnace melting and annealing at 1100 K [9]. It was characterized by X-ray diffraction (XRD), energy dispersive analysis of X-rays and differential scanning calorimetry [16]. The atomically clean specimen surface was prepared by in situ scraping using a diamond file and the chamber base pressure was 6 × 10$^{-11}$ mbar. UPS was performed with a He I ($h\nu = 21.2$ eV) photon source using electron energy analyzer from Specs GmbH, Germany. The overall resolution was 120 meV.

Mn$_2$NiGa has a cubic $L_2_1$ structure in the austenitic phase that consists of four interpenetrating f.c.c. lattices at $(0,0,0)$, $(0.25,0.25,0.25)$, $(0.5,0.5,0.5)$, and $(0.75,0.75,0.75)$ (fig. 1a) [11,16]. The structure of Mn$_2$NiGa can be better explained in comparison to Ni$_2$MnGa that also has $L_2_1$ structure. In Ni$_2$MnGa, the Ni atoms are at $(0.25,0.25,0.25)$ and $(0.75,0.75,0.75)$, while Mn and Ga are at $(0.5,0.5,0.5)$ and $(0.0,0)$, respectively and there is no direct Mn-Mn interaction, with Mn having eight Ni atoms as nearest neighbours. In contrast, Mn$_2$NiGa has one Mn atom at $(0.5,0.5,0.5)$ (referred to as MnII), while the other Mn atom (MnI) occupies the Ni atom position $(0.75,0.75,0.75)$ of Ni$_2$MnGa. Thus, MnI and MnII occupy inequivalent sites in the unit cell, and there is a direct Mn-Mn interaction since MnI and MnII are nearest neighbours. In the martensitic phase, the XRD pattern for Mn$_2$NiGa has been indexed by a tetragonal unit cell with $c/a = 1.21$ (fig. 1b) [11,16].

**Total energy and magnetic moment calculation.** – To determine whether minimization of $E_{tot}$ causes the structural transition, we have calculated $E_{tot}$ for both phases as a function of the lattice parameters in the lowest-energy magnetic state (discussion about the magnetic state is given later). In the austenitic phase, $E_{tot}$ as a function of cell volume ($V$) exhibits a parabolic behaviour and the minimum (shown by the arrow) determines the optimized lattice constant ($a = 11.059$ a.u. = 5.85 Å) (fig. 2a). The agreement is within 1% of the experimental value of 5.9072 Å [11]. For the martensitic phase, in the first step, $E_{tot}(V)$ is calculated to obtain optimized $V = 1330$ a.u.$^3$ at fixed $c/a = 1.21$ (XRD value). Next, $E_{tot}(c/a)$ is calculated at $V = 1330$ a.u.$^3$. This gives the optimized $c/a$ to be 1.25. In the final step, $E_{tot}(V)$ is calculated again with $c/a = 1.25$ (fig. 2a). A least-square fitting of the data [8,23] gives the $E_{tot}$ minimum at 1335.2 a.u.$^3$ (shown by the arrow). From fig. 2a, the $E_{tot}$ minimum in the martensitic phase is 6.8 meV/atom lower than the austenitic phase. This demonstrates that the martensitic phase is stabilized through a sizable

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Fig. 1: (Color online) The structure of Mn$_2$NiGa in the (a) austenitic and (b) martensitic phase; the blue, green, red, and brown spheres represent Ni, MnI, MnII and Ga, respectively.

Fig. 2: (Color online) (a) The calculated total energies ($E_{tot}$) of Mn$_2$NiGa as a function of the cell volume of the austenitic and martensitic phase. (b) Three-dimensional plot of the spin magnetic-moment distribution (in unit of eA$^{-3}$) in the (110)-plane in the martensitic phase, a contour plot is shown in the bottom.
tetragonal distortion \((c/a = 1.25)\). The optimized lattice constants \((a = 5.409\) and \(c = 6.762, \text{Å}\) are within \(2.1\%\) and \(0.85\%\) of the experimental lattice constants \(a = 5.5272\) Å and \(c = 6.7044\) Å, respectively [11]. Thus, the agreement of the lattice constants for both the phases is satisfactory, considering that even for free-electron–like non-magnetic metals there could be about \(2\%\) discrepancy between experiment and GGA-based DFT theory [24]. The decrease of \(V\) by \(1.2\%\) is in agreement with the experimental volume decrease of \(0.64\%\) in the martensitic phase [11].

The lowest-energy magnetic state is obtained by performing \(E_{\text{tot}}\) minimization over various possible starting MnI and MnII magnetic-moment combinations, as discussed in details in ref. [25]. For both the austenitic and martensitic phase, the anti-parallel starting spin (equal or unequal) configurations of MnI and MnII converge to a ferrimagnetic state that has minimum \(E_{\text{tot}}\). We have used the starting Mn magnetic moments for structure optimization runs to be \(3\mu_B\) for both Mn atoms in anti-parallel orientation. However, when the starting MnI and MnII moments are parallel (equal or unequal), \(E_{\text{tot}}\) converges to different magnetic moments related to local minima at higher energies. For example, in the austenitic phase there are three local minima [25]. Also in the martensitic phase, multiple local minima are obtained with parallel starting moments of MnI and MnII. In particular, a local minimum that is \(108\) meV/atom higher in \(E_{\text{tot}}\), gives MnI and MnII moments to be 0.24 and \(3.1\) \(\mu_B\) [25]. Thus, one Mn moment is small, as has been reported in ref. [14]. Our calculation based on the magnetic moments reported in ref. [14] converges at \(193\) meV/atom higher energy than the \(E_{\text{tot}}\) minimum [25]. This gives an idea why the results from ref. [14] are in disagreement with experimental data, as discussed later.

The spin magnetic-moment distribution in the martensitic phase clearly shows that it is ferrimagnetic with MnI magnetic-moment anti-parallel and smaller than MnII (fig. 2b). The Ni moment is small and is parallel to the Mn moment. For the martensitic (austenitic) phase, the local spin magnetic moments are \(-2.21\) \((-2.43)\), \(2.91\) \((3.2)\), \(0.27\) \((0.32)\), \(0.01\) \((0.01)\) \(\mu_B\) per formula unit \((\mu_B/f.u.)\) for MnI, MnII, Ni, and Ga, respectively. The moment related to the interstitial charge is small \((-0.04\mu_B)\). The total moment for the martensitic phase \((1.01\mu_B/f.u.)\) is \(11\%\) less than the austenitic phase \((1.14\mu_B/f.u.)\). The lowering of the magnetic-moment in the martensitic phase has been reported by Liu et al. from magnetization studies: \(2.12\mu_B/f.u.\) \((28.28\text{emu/g})\) and \(1.29\mu_B/f.u.\) \((30.33\text{emu/g})\) in the martensitic and austenitic phase, respectively [11]. Thus, the magnetic-moment values and the trend that magnetization is lower in the martensitic phase are in agreement with our calculations.

**Density of states and photoemission spectroscopy.** The stabilization of the tetragonally distorted martensitic phase in \(\text{Ni}_2\text{MnGa}\) has been related to the band Jahn-Teller effect, where a DOS peak at \(E_F\) in the cubic phase splits into two peaks below and above \(E_F\) in the tetragonal phase, resulting in a lowering of the total energy [17]. Splitting and shift of the DOS peaks just below \(E_F\) have also been observed in \(\text{Ni}_{2.25}\text{Mn}_{0.75}\text{Ga}\) [9]. For \(\text{Mn}_2\text{NiGa}\), the differences in the total DOS near \(E_F\) are interesting: a peak at \(-0.1\) eV in the austenitic phase shifts to lower energy \((-0.35\) eV) and diminishes in intensity in the martensitic phase (both peaks indicated by arrows). The peak above \(E_F\) at \(0.35\) eV (tick) does not shift but is enhanced in intensity in the martensitic phase indicating a transfer of DOS from the occupied to the unoccupied states. From the partial DOS (PDOS), it is clear that the peaks at \(-0.1\) and \(-0.35\) eV arise primarily due to Ni 3d and Mn 3d hybridization. The shift of the \(-0.1\) eV peak to lower energy in the martensitic phase results from the enhanced Ni 3d- Mn 3d hybridization caused by a decrease in the Ni-Mn distance from \(2.925\) Å (austenitic) to \(2.701\) Å (martensitic) and is a possible reason for the stabilization of the martensitic phase. The DOS at \(E_F\) is substantially reduced in the martensitic phase \((1.29\) states/eV f.u.) compared to the austenitic phase \((3.39)\). Thus, a decrease in the electronic specific heat in the martensitic phase could be expected.

The antiferromagnetic alignment of MnI and MnII spin moments can be understood from the 3d spin resolved PDOS (fig. 3b). MnI 3d minority-spin states appear below \(E_F\) between \(-1\) and \(-3.5\) eV, whereas MnII 3d majority-spin states appear below \(E_F\) with two well-separated high-PDOS regions around \(-1.5\) and \(-2.7\) eV. MnI 3d majority-spin states appear primarily above \(E_F\) centered around \(0.7\) eV; while MnII 3d minority-spin states appear above \(E_F\) with the main peak at \(1.1\) eV and a smaller peak at \(0.35\) eV. Thus, while the minority-spin
states are mostly excluded from the MnII 3d shell, the majority-spin states are excluded from the MnI 3d shell resulting in large but oppositely aligned moments. MnI and MnII are nearest neighbors (n.n.) with a n.n. distance of 2.549 (2.533) Å in the martensitic (austenitic) phase. The exchange pair interaction as a function of Mn-Mn separation was calculated by a Heisenberg-like model and an antiferromagnetic coupling at short interatomic distances was found that becomes ferromagnetic at larger distances [12]. Thus, the direct Mn-Mn interaction at short interatomic distance is responsible for their opposite alignment [12,13]. The energy separation between the centroid of the occupied and the unoccupied spin states of opposite polarization gives an exchange splitting of 2.7 eV (3.1 eV) for MnI (MnII) in the martensitic phase. In the austenitic phase, the exchange splittings are 2.8 and 2.7 eV (3.1 eV) for MnI (MnII) in the martensitic phase. The energy separation between the majority-spin Ni and MnII 3d states is highest.

It was shown for Mn excess Ni2Mn1+xGa1−x that the magnetic moments of the Mn atom in the Ga site is equal but anti-parallel to the Mn atom at the Mn site [26]. This would tend to suggest that in Mn2NiGa, the Mn moments would cancel and a small total moment might result from Ni. However, this does not happen and the difference of MnI and MnII moments is a key to the larger total moment (≈1 µB). This originates from the stronger hybridization between the majority-spin Ni and MnII 3d states in comparison to hybridization between Ni and MnI 3d minority-spin states. Note that Ni and MnII are n.n. separated by 2.549 (2.533) Å in the martensitic (austenitic) phase and stronger hybridization pulls down almost all the MnII 3d majority-spin states below $E_F$ resulting in strong spin polarization and larger moment. On the contrary, hybridization between Ni and MnI 3d minority-spin states is relatively weaker, distance being larger: 2.701 (2.925) Å in the martensitic (austenitic) phase, and there are sizable MnI 3d minority-spin states above $E_F$ including the 0.35 eV peak, resulting in smaller moment on MnI.

Photoemission spectroscopy is a direct probe of the DOS in the VB region. In fig. 4, the main peak of the UPS VB spectrum appears at −1.4 eV and the Fermi cutoff is at 0 eV. In order to calculate the VB spectrum, we note that because of the order of magnitude larger photoemission cross-sections of Ni 3d and Mn 3d (4.0 and 5.3 mega barns at $hν = 21.2$ eV, respectively) [27], these PDOS determine the shape of VB [28]. So, we have added the Ni and Mn 3d PDOS in proportion to their cross-sections, multiplied by the Fermi function and broadened by the instrumental Gaussian resolution and the lifetime-width–related energy-dependent Lorenzian to obtain the calculated VB (fig. 4). This is a standard procedure of comparing the photoemission spectrum from a polycrystalline sample with the calculated DOS [28,29]. The position of the main peak at −1.4 eV and the ratio between the main peak and the intensity at $E_F$ are in good agreement with UPS VB spectrum. It is clear from fig. 4 that the main peak is dominated by Mn 3d-Ni 3d hybridized states that have almost equal contribution. States near $E_F$ are dominated by Mn 3d states, and the MnI 3d in particular.

The martensitic phase DOS from ref. [14], obtained by adding up the majority and minority-spin DOS from fig. 5 of ref. [14], is in clear disagreement with our DOS (fig. 3a). This prompted us to calculate the VB spectrum from the PDOS of ref. [14] following the same procedure as discussed above and compare it with the experimental UPS VB. As shown in fig. 4, the calculated VB based on ref. [14] is in obvious disagreement with UPS VB: no clear peak is observed in the former; a weak broad feature is present at −2 eV and the intensity near $E_F$ is highest. This shows that the martensitic phase DOS reported in ref. [14] is inconsistent with experiment. Moreover, the large change of local moments (austenitic MnI $≈$−2.2, MnII = 3.15, Ni 0.27 µB to martensitic MnI $≈$0, MnII = 1.4 µB) obtained in ref. [14] is physically unexpected [25], since the MnI-MnII distance changes by only 0.6% in the martensitic phase. Thus, it is no wonder why the total moment reported in ref. [14] is higher in the martensitic phase compared to the austenitic phase, in contradiction to their own magnetization data [11,14].

![Fig. 4: (Color online) UPS valence band (VB) spectrum of Mn2NiGa in the martensitic phase compared with the theoretical VB spectrum calculated from the DOS in fig. 3a. The contributions from the Mn 3d and the Ni 3d partial DOS are also shown. The spectra have been shifted along the vertical axis for clarity of presentation.](image)

**Electronic bands and Fermi surface.**

**Austenitic-phase majority-spin states.** We now turn to the discussion of the electronic bands and Fermi surface of Mn2NiGa. The majority-spin bands in the austenitic phase show that band 29 forms electron pockets (fig. 5b). The corresponding FS, shown in fig. 5d, is distorted prolate ellipsoidal in shape and occurs around the X point of the Brillouin zone (BZ) with the long axis along the
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Table 1: Nesting vectors for the Fermi surface of Mn$_2$NiGa, in units of $2\pi/a$ (= 1 a.u.).

| Band no. | Austenitic phase | Martensitic phase |
|----------|------------------|-------------------|
|          | Majority spin    | Minority spin     | Majority spin | Minority spin |
| Band 29  | 0.44(1,0,0), 0.44(0,1,0) | –                  | 0.34(1,0,0)   | 0.34(0,1,0)   |
| Band 28  | –                 | 0.31{1,0,0}       | 0.75(1,1,0), 0.75(1,−1,0), 1.13(0,0,1) | – |
| Band 27  | –                 | 0.4{1,0,0}        | –             | – |

Fig. 5: (Color online) (a) The f.c.c. Brillouin zone showing the high symmetry directions. (b) Majority- and (c) minority-spin energy bands of Mn$_2$NiGa in the austenitic phase. Majority-spin Fermi surface (FS) of the (d) austenitic phase compared to the (e) martensitic phase FS related to bands 28 and 29. Minority-spin austenitic phase FS related to (f) band 27 and (h) band 28. Insets show the FS in a different orientation. Martensitic phase minority-spin FS related to (g) band 27 and (i) band 28. All the FS are shown in the repeated zone scheme and yellow arrows represent the nesting vectors. Black arrows relate the FS of the two phases.

\[ \Gamma X \] direction. The BZ is shown in fig. 5a. The projection of the FS along \( \Gamma X \) is a square (inset, fig. 5d), which indicates that FS nests onto itself with n.v. 0.44(1,0,0) and 0.44(0,1,0), in units of $2\pi/a$ (= 1 a.u.). The nested portion of the FS is a rhombus (shown by black lines in fig. 5d) of area 0.052 a.u.$^2$ with an opening angle of about 15°.

**Martensitic-phase majority-spin states.** In the martensitic phase, the majority-spin FS exhibits interesting modification (fig. 5e). The majority-spin band-29-related electron-type FS is now connected as continuous pipes along the (1,0,0) direction, but with varying cross-section with flat parallel parts that nest onto each other (green/pink online sheet in fig. 5e). The n.v. are 0.34(1,0,0) and 0.34 (0,1,0), and compared to the austenitic phase the direction is the same but the magnitude of the n.v.'s is reduced. Interestingly, a second majority-spin band (28) crosses \( E_F \) that results in a hole-type cuboid FS around the \( \Gamma \)-point that has no counterpart in the austenitic phase (blue online sheet, fig. 5e). Two mutually perpendicular n.v.'s 0.75(1,1,0) and 0.75(1,−1,0) are identified, along with a larger n.v. of 1.13(0,0,1). The n.v.'s along the \{1,0,0\}, identified above, are not expected to contribute to phonon softening because these hardly contribute to the electron-phonon coupling matrix element [19]. On the other hand, the 0.75(1,1,0) and 0.75(1,−1,0) n.v.'s might be responsible for the softening of the TA$_{2}[110]$ phonon resulting in a modulated martensitic phase. The different nesting vectors are shown in table 1.

From figs. 5d and e, the majority-spin FS is clearly enlarged in the martensitic phase compared to the austenitic phase. On the contrary, for the minority-spin states (figs. 5f–i), the FS clearly shrinks in the martensitic phase.

**Austenitic-phase minority-spin states.** In the austenitic phase, the minority-spin band 27 is hole-type dispersing above (below) \( E_F \) at 0.2TL (0.5LW) and generates a distorted cubic FS, where one pair of diagonally opposite corners taper out (fig. 5f). FS nesting is observed between the cube faces with n.v. 0.4\{1,0,0\}, as shown by the yellow online arrows. The second sheet of the FS (band 28) is electron-like, consisting of multiply connected pipes of square cross-section (inset, fig. 5h). The parallel surfaces of the pipes nest onto each other with a n.v. of 0.31\{1,0,0\} a.u. and a nesting area of 0.16 a.u.$^2$.

**Martensitic-phase minority-spin states.** In the martensitic phase, the minority-spin hole-type FS (band 27)
has a flower-like shape with a perforation in the middle (fig. 5g). The electron-type FS sheet shrinks to disconnected pipes of varying diameter (fig. 5i). These minority-spin FS sheets (figs. 5g, i) in the martensitic phase do not exhibit nesting.

**Conclusion.** — We observe a FS nesting in the martensitic phase along the [1,1,0] direction in the majority-spin FS that might lead to the instability of the TA2 phonon mode in Mn$_2$NiGa. The austenitic phase FS is drastically modified in the martensitic phase. The majority-spin FS expands in the martensitic phase, while the minority-spin FS shrinks. We show that Mn$_2$NiGa is an itinerant ferromagnet in both the austenitic and martensitic phase, and that the MnII or Ni moments do not become zero in the martensitic phase, refuting a recent work by Liu et al. [14]. The unequal-spin magnetic moments in the two inequivalent Mn atoms (MnI and MnII) arise from the different in the hybridization of the MnI 3d-Ni 3d and MnII 3d-Ni 3d states, which in turn is related to the interatomic distances. We furthermore show that in Mn$_2$NiGa a large tetragonal distortion ($c/a = 1.25$) decreases the total energy, stabilizing the lower-temperature martensitic phase. Mn$_2$NiGa would be an ideal system to study different models of magnetization in metals, since it has a simple $L_2_1$ structure and three sublattice magnetization with parallel (between MnII and Ni) and anti-parallel (between MnI and MnII) magnetic-moment alignment. Possibility of incommensurate magnetic phase or charge density wave instabilities could be expected at low temperatures due to the presence of FS nesting and ferrimagnetism. Low-temperature X-ray diffraction might be able to detect possible occurrence of a charge density wave state. Neutron scattering, angle-resolved photoemission or Compton scattering experiments can verify the theoretically predicted FS. In fact, FS nesting, ferrimagnetism and large magnetoelastic coupling makes Mn$_2$NiGa a highly interesting material that has remained largely unexplored so far.

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We thank K. Kunc and A. De Sarkar for fruitful discussions. P. Chaddah, V. C. Sahni, K. Horn, A. Gupta and S. M. Oak are thanked for support. Ramanna Fellowship Research Grant and D.S.T.-Max Planck Partner Group Project are thanked for funding.

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