Supporting Information

for

Structure and spin-glass magnetism of the $Fe_{1.5}Ni_{1.5}Ga_4$ metallic alloy

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1. *hk*0 and *hhl* planes in the reciprocal space constructed from the SCXRD data collected for the $Fe_{1.5}Ni_{1.5}Ga_4$ crystal.

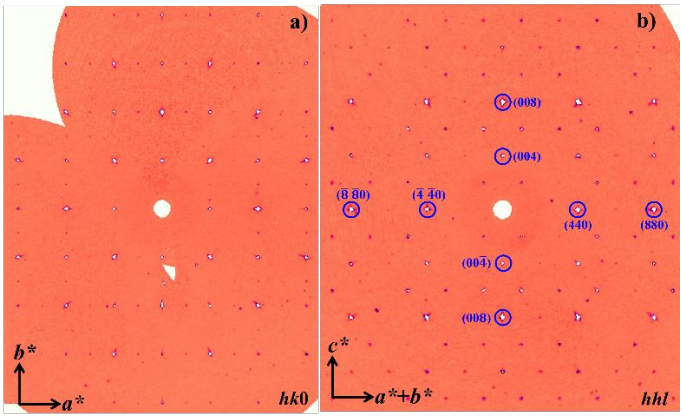


Figure S1. (a) *hk*0 and (b) *hhl* planes in the reciprocal space constructed from the SCXRD data collected for the $Fe_{1.5}Ni_{1.5}Ga_4$ crystal. The reflections corresponding to $h + k + l = 2n$ are encircled in blue.

2. EDS elemental maps of the $Fe_{1.5}Ni_{1.5}Ga_4$ material.

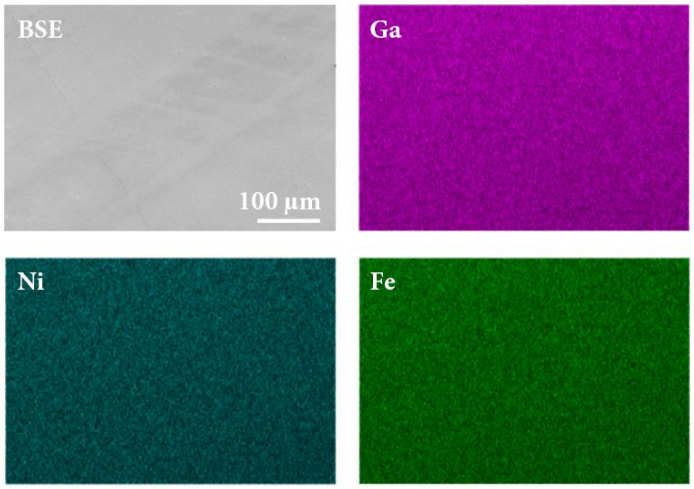
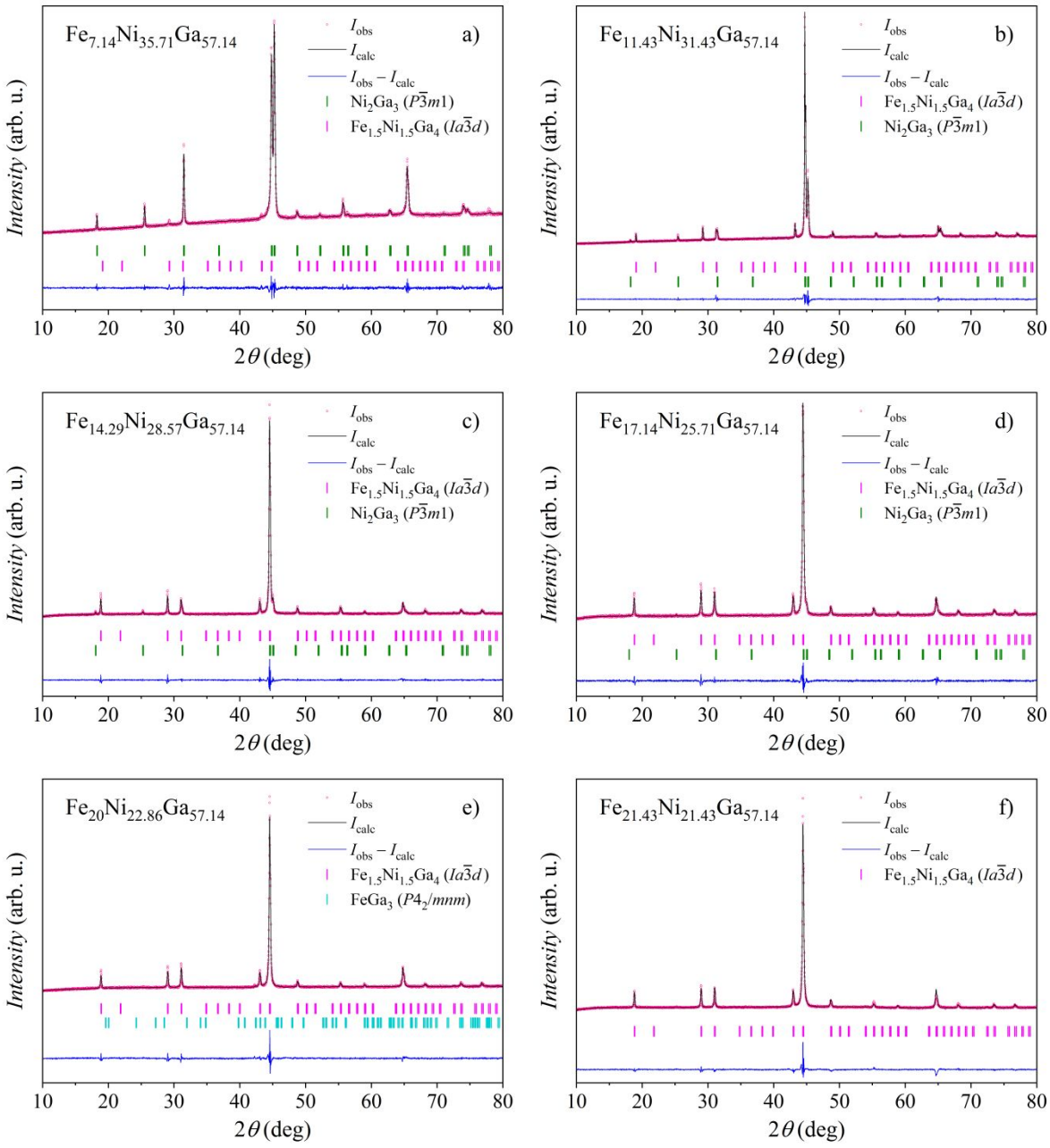


Figure S2. EDS elemental maps of the $Fe_{1.5}Ni_{1.5}Ga_4$ material. The SEM backscattered-electron (BSE) image of the same area is shown in the upper left panel.

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3. Refinement diffractograms (either Rietveld or Le Bail) and refinement details of PXRD data of ten $Fe_xNi_{3-x}Ga_4$ compositions along a constant Ga line (57.14 at.% of Ga).



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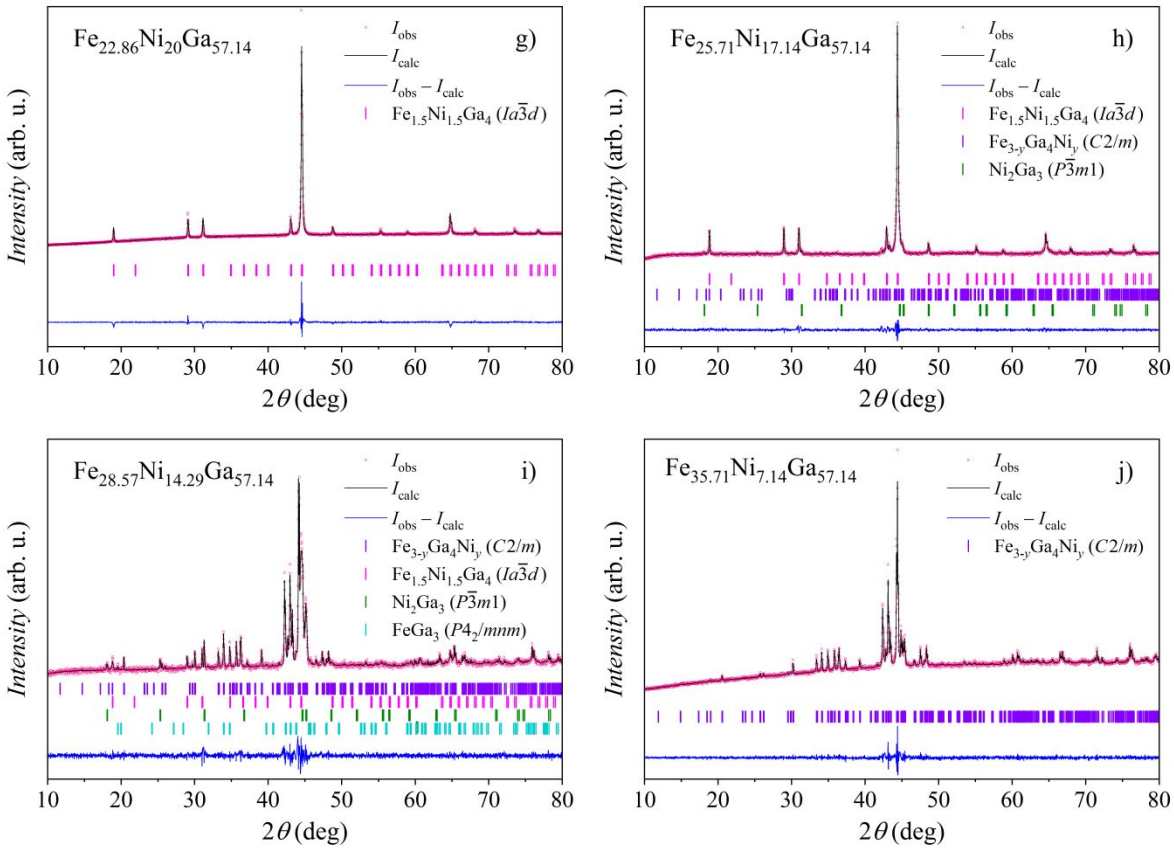


Figure S3. Refinement diffractograms (either Rietveld or Le Bail) of PXRD data of ten $Fe_xNi_{3-x}Ga_4$ compositions along a constant Ga line (57.14 at.% of Ga). The loading compositions (in at.%) with nominal Fe contents x = 0.5, 0.8, 1.0, 1.2, 1.4, 1.5, 1.6, 1.8, 2.0 and 2.5 are written in the top left corner of each panel. Bragg positions of the phases present in each composition are shown by tick marks (in different color for each phase) and are ordered according to their presence (the top trace is the major phase). The refinement parameters for each composition are given in Table S1.

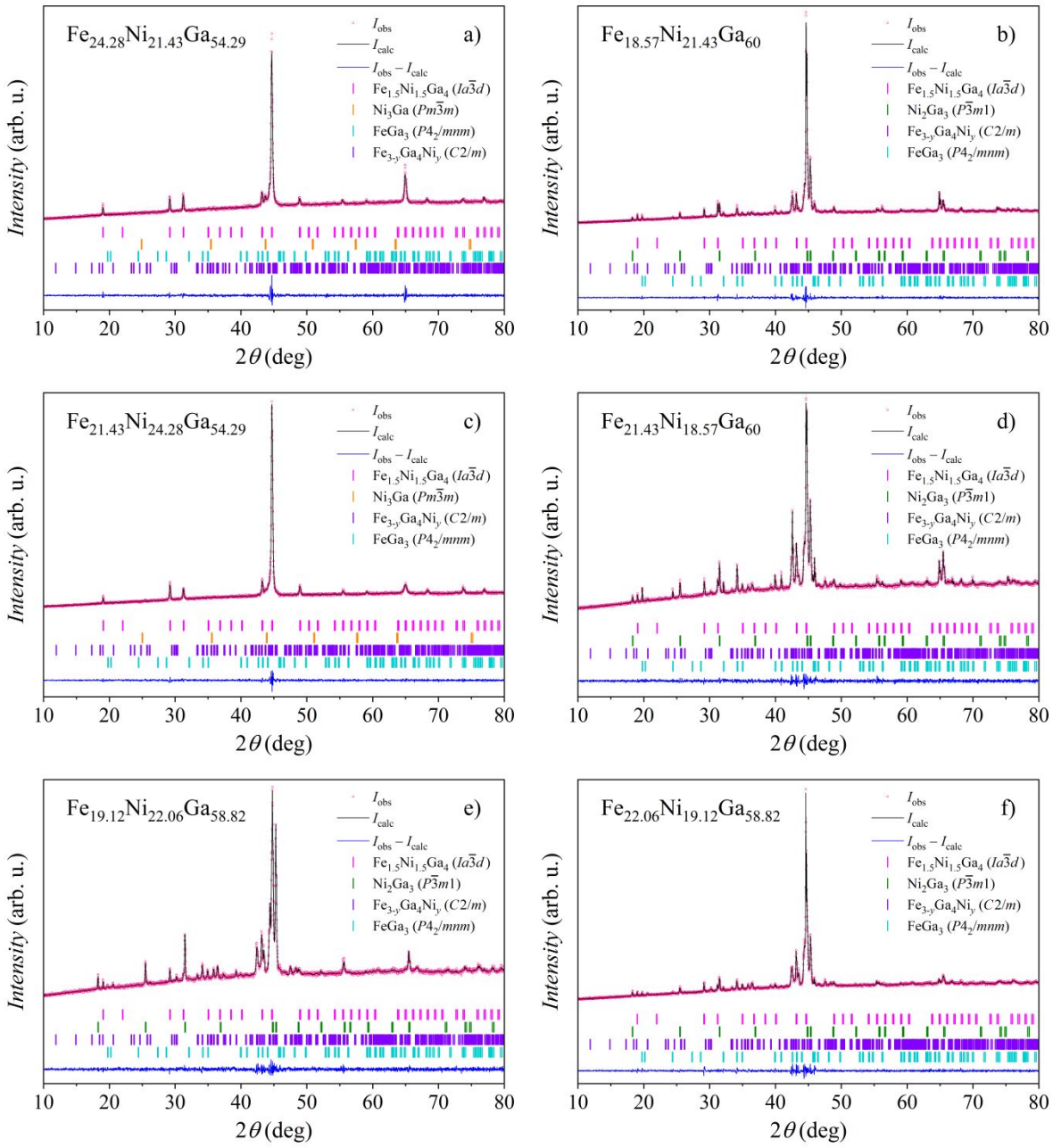
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Table S1. Refinement details of the $Fe_xNi_{3-x}Ga_4$ samples. For each composition, the major phase is denoted as P1, while other phases are denoted as P2, P3, and P4 (with decreasing presence).

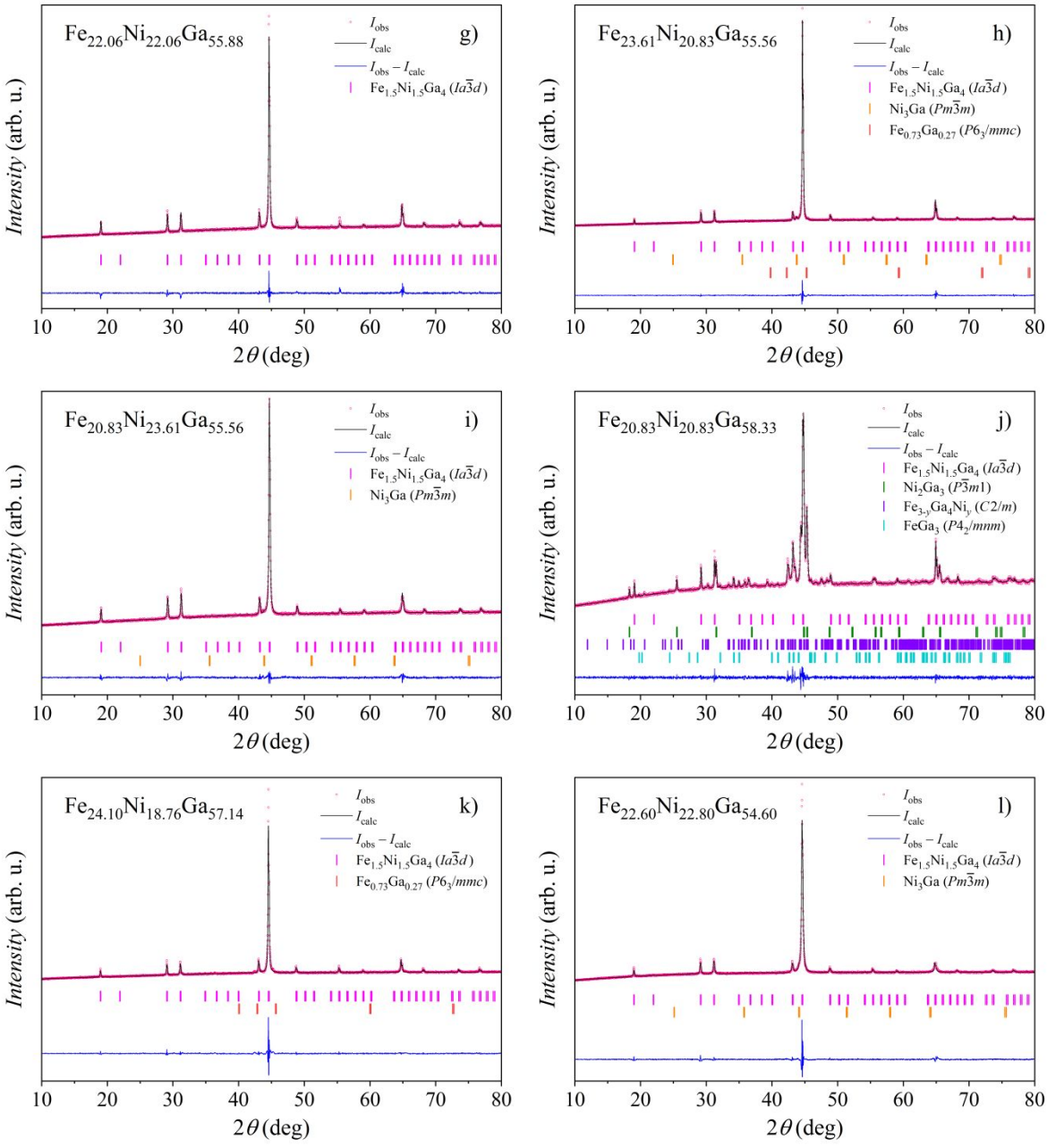
Composition (at.%)			Phases	Refinement method	Refinement parameters
Fe	Ni	Ga			
7.14	35.71	57.14	P1: Ni_2Ga_3 ($P\bar{3}m1$) P2: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$)	Le Bail	GOF =1.29, R_p = 0.0293, wR_p = 0.0385
11.43	31.43	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$)	Le Bail	GOF =1.45, R_p = 0.0305, wR_p = 0.0417
14.29	28.57	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$)	Le Bail	GOF =1.53, R_p = 0.0221, wR_p = 0.0307
17.14	25.71	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$)	Le Bail	GOF =1.43, R_p = 0.0211, wR_p = 0.0288
20.00	22.86	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.53, R_p = 0.0242, wR_p = 0.0335
21.43	21.43	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$)	Rietveld	GOF =1.88, R_p = 0.0189, wR_p = 0.0292
22.86	20.00	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$)	Rietveld	GOF =1.68, R_p = 0.0302, wR_p = 0.0443
25.71	17.14	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P3: Ni_2Ga_3 ($P\bar{3}m1$)	Le Bail	GOF =1.22, R_p = 0.0194, wR_p = 0.0252
28.57	14.29	57.14	P1: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P2: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P3: Ni_2Ga_3 ($P\bar{3}m1$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.39, R_p = 0.0213, wR_p = 0.0291
35.71	7.14	57.14	P1: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$)	Le Bail	GOF =1.27, R_p = 0.0239, wR_p = 0.0319

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4. Refinement diffractograms (either Rietveld or Le Bail) and refinement details of PXRD data of fourteen $Fe_xNi_yGa_z$ compositions ($1.3 \leq x \leq 1.74$, $1.26 \leq y \leq 1.7$ and $3.8 \leq z \leq 4.2$).



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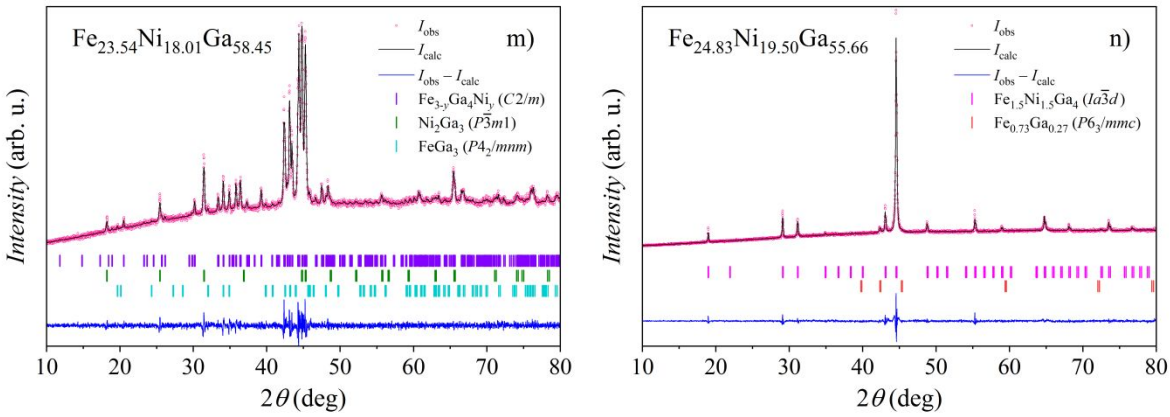


Figure S4. Refinement diffractograms (either Rietveld or Le Bail) of PXRD data of fourteen $Fe_xNi_yGa_z$ compositions ($1.3 \leq x \leq 1.74$, $1.26 \leq y \leq 1.7$ and $3.8 \leq z \leq 4.2$). The loading compositions (in at.%) are written in the top left corner of each panel. Bragg positions of the phases present in each composition are shown by tick marks (in different color for each phase) and are ordered according to their presence (the top trace is the major phase). The refinement parameters for each composition are given in Table S2.

Table S2. Refinement details of the $Fe_xNi_yGa_z$ samples, where the Ga composition was tuned along with the Fe and Ni. For each composition, the major phase is denoted as P1, while other phases are denoted as P2, P3, and P4 (with decreasing presence).

Composition (at.%)			**Phases**	**Refinement method**	**Refinement parameters**
Fe	Ni	Ga			
24.28	21.43	54.29	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_3Ga ($Pm\bar{3}m$) P3: $FeGa_3$ ($P4_2/mnm$) P4: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$)	Le Bail	GOF =1.28, R_p = 0.0280, wR_p = 0.0378

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18.57	21.43	60.00	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$) P3: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.32, R_p = 0.0272, wR_p = 0.0366
21.43	24.28	54.29	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_3Ga ($Pm\bar{3}m$) P3: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.15, R_p = 0.0263, wR_p = 0.0340
21.43	18.57	60.00	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$) P3: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.16, R_p = 0.0242, wR_p = 0.0317
19.12	22.06	58.82	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$) P3: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.15, R_p = 0.0250, wR_p = 0.0320
22.06	19.12	58.82	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$) P3: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.46, R_p = 0.0271, wR_p = 0.0376
22.06	22.06	55.88	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$)	Rietveld	GOF =1.57, R_p = 0.0300, wR_p = 0.0441
23.61	20.83	55.56	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_3Ga ($Pm\bar{3}m$) P3: $Fe_{0.73}Ga_{0.27}$ ($P6_3/mmc$)	Le Bail	GOF =1.41, R_p = 0.0260, wR_p = 0.0354
20.83	23.61	55.56	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_3Ga ($Pm\bar{3}m$)	Le Bail	GOF =1.29, R_p = 0.0264, wR_p = 0.0356

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20.83	20.83	58.33	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_2Ga_3 ($P\bar{3}m1$) P3: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P4: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.26, R_p = 0.0218, wR_p = 0.0293
24.10	18.76	57.14	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: $Fe_{0.73}Ga_{0.27}$ ($P6_3/mmc$)	Le Bail	GOF =1.81, R_p = 0.0290, wR_p = 0.0421
22.60	22.80	54.60	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: Ni_3Ga ($Pm\bar{3}m$)	Le Bail	GOF =1.73, R_p = 0.0247, wR_p = 0.0367
23.54	18.01	58.45	P1: $Fe_{3-y}Ga_4Ni_y$ ($C2/m$) P2: Ni_2Ga_3 ($P\bar{3}m1$) P3: $FeGa_3$ ($P4_2/mnm$)	Le Bail	GOF =1.34, R_p = 0.0247, wR_p = 0.0328
24.83	19.50	55.66	P1: $Fe_{1.5}Ni_{1.5}Ga_4$ ($Ia\bar{3}d$) P2: $Fe_{0.73}Ga_{0.27}$ ($P6_3/mmc$)	Le Bail	GOF =1.45, R_p = 0.0297, wR_p = 0.0403

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