Spin wave and phonon dispersion in Fe-Ga solid solutions

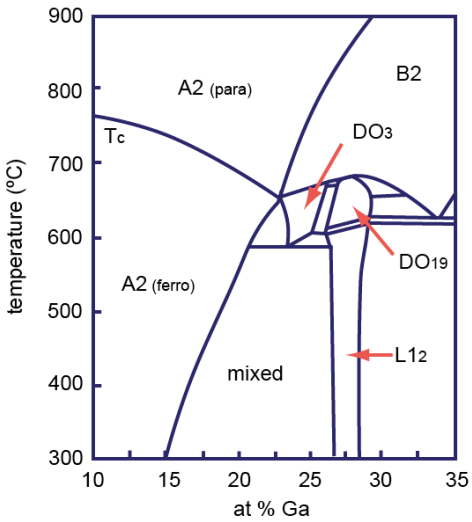
Fe-Ga alloys with appropriate composition and heat treatment, exhibit giant magnetostriction in a polycrystalline and ductile form.[1,2] The tetragonal magnetostriction coefficient, λ_{100}, of Fe-Ga can be up to 15 times that of pure Fe. This makes these materials of tremendous scientific interest as well as technological interest for use in devices such as actuators, transducers and sensors. Elastic constant measurements[3] show that the shear elastic constant $1/2(C_{11}-C_{12})$ decreases with increasing Gallium concentration and extrapolates to zero at approximately 26 at.% Ga. The slope of the phonon dispersion curve at low-q of the T_2[110] branch is a measure of that elastic constant and hence the interest in measuring phonons in these materials. With the large magnetoelastic interactions in such a material, it is also of interest to measure the spin wave dispersion.
In the neutron school experiments at HB1A and HB3, we will use samples of two compositions of Fe-Ga alloys in to measure both phonon and spin wave neutron groups at room temperature.

[1]A. E. Clark, K. B. Hathaway, M. Wun-Fogle, J. B. Restorff, T. A. Lograsso, V. M. Keppens, G. Petculescu, and R. A. Taylor, J. Appl. Phys., 93, 8621 (2003).
[2] G. Petculescu, K. B. Hathaway, T. A. Lograsso, M. Wun-Fogle, and A. E. Clark, J. Appl. Phys., 97, 10M315 (2005).
[3] M. Wuttig, L. Dai, and J. R. Cullen, Appl. Phys. Let., 80, 1135 (2002).

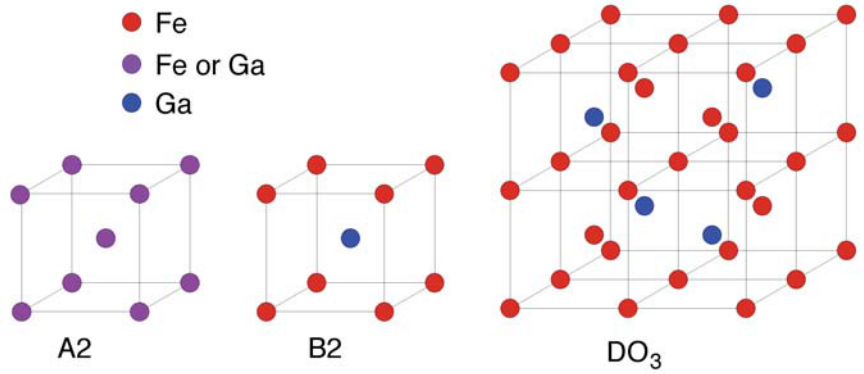
General references on inelastic neutron scattering;
Neutron Diffraction, Oxford University (1975), G. E. Bacon
Neutron Scattering with a Triple-Axis Spectrometer, Cambirdge University (2002), G.Shriane, S.M.Shapiro, J.M.Tranquada.

References more specific to the sample materials;
"Phonon Dispersion Relation for Iron," V.J.Minkiewicz, G.Shirane, R. Nathans, Phys.Rev., **162**, 528 (1967).
"Neutron Scattering Investigation of the Magnetic Excitations in Iron," H.A.Mook, R.M.Nicklow, Phys. Rev. B, **7**, 336, (1973).
"Spin-wave dispersion in magnetostrictive Fe-Ga alloys: Inelastic neutron scattering measurements," J. L. Zarestky, O. Moze, J. W. Lynn, Y. Chen, D. L. Schlagel, T. A. Lograsso, Phys. Rev. B, **75**, 052406-1 (2007).
"Compositional variation of the phonon dispersion curves of bcc Fe-Ga alloys", J. L. Zarestky, V. O. Garlea, T. A. Lograsso, D. L. Schlagel and C. Stassis, Phys.Rev.B, **72**, 180408(R) (2005).

Data analysis links SPICE web page; http://neutron.ornl.gov/spice/ download Graffiti, the application that reads and plots SPICE data files. (Mac version at; http://www.ornl.gov/~jxz/alns/index.html about 2/3 of the way down the page)

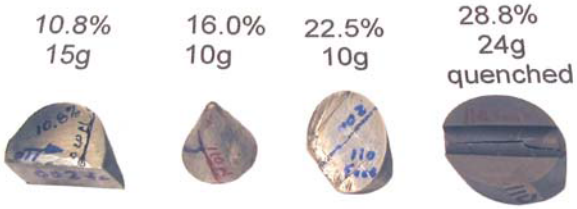


Phase diagram of Fe-Ga system.
O. Ikeda, et al., *J. Alloys Comp.,* **347**, 198 (2002).



Fe-Ga structures

Fe-Ga samples;



Fe-Ga A2 structure crystallographic information;

****
* Output generated by CrystalDiffract *
* © 1995-2002 David C Palmer, < D.C.Palmer@CrystalMaker.co.uk > *
* CrystalDiffract is a powder diffraction module for *
* CrystalMaker - interactive crystallography for MacOS *
* http://www.crystalmaker.co.uk *
****

UNIT CELL DATA
a = 2.9000; b = 2.9000; c = 2.9000 Angstroms
alpha = 90.000; beta = 90.000; gamma = 90.000 degrees
cell volume = 24.389 A**3
calculated density = 8030.21 kg / m**3

RECIPROCAL UNIT CELL DATA
a* = 0.3448; b* = 0.3448; c* = 0.3448 Reciprocal Angstroms
alpha* = 90.000; beta* = 90.000; gamma* = 90.000 degrees

Lattice type = I
ASYMMETRIC UNIT

label	------- Site Occupancy -------		x	y	z	Num In Cell
Fe1	Fe	0.775	0.0000	0.0000	0.0000	2
Ga1	Ga	0.225	0.0000	0.0000	0.0000	2

Total of: 4 atoms in the unit cell

REFLECTIONS LIST
Neutron wavelength = 2.3560 A
Notes:
1. Intensities are relative to 1 cubic Angstrom of material
2. multiplicities may show unexpected values if two reflections
with different sets of Miller Indices have the same d-spacing.
In these cases, CrystalDiffract lists the SUM of the multiplicities
for all reflections with the same d-spacing

ref no.	(N)	h	k	l	d(hkl)	2-Theta	Intensity	I/Imax	m(hkl)
[1]	2	1	1	0	2.05061	70.1241	1.70808e+01	10.4	12
[2]	4	2	0	0	1.45000	108.6649	5.92375e+00	3.6	6
[3]	6	1	2	1	1.18392	168.5354	1.63997e+02	100.0	24

Fe-Ga DO_3 structure crystallographic information;

****
* Output generated by CrystalDiffract *
* © 1995-2002 David C Palmer, < D.C.Palmer@CrystalMaker.co.uk > *
* CrystalDiffract is a powder diffraction module for *
* CrystalMaker - interactive crystallography for MacOS *
* http://www.crystalmaker.co.uk *
****

UNIT CELL DATA
a = 5.8000; b = 5.8000; c = 5.8000 Angstroms
alpha = 90.000; beta = 90.000; gamma = 90.000 degrees
cell volume = 195.112 A**3
calculated density = 12824.42 kg / m**3

RECIPROCAL UNIT CELL DATA
a* = 0.1724; b* = 0.1724; c* = 0.1724 Reciprocal Angstroms
alpha* = 90.000; beta* = 90.000; gamma* = 90.000 degrees

Lattice type = F
ASYMMETRIC UNIT

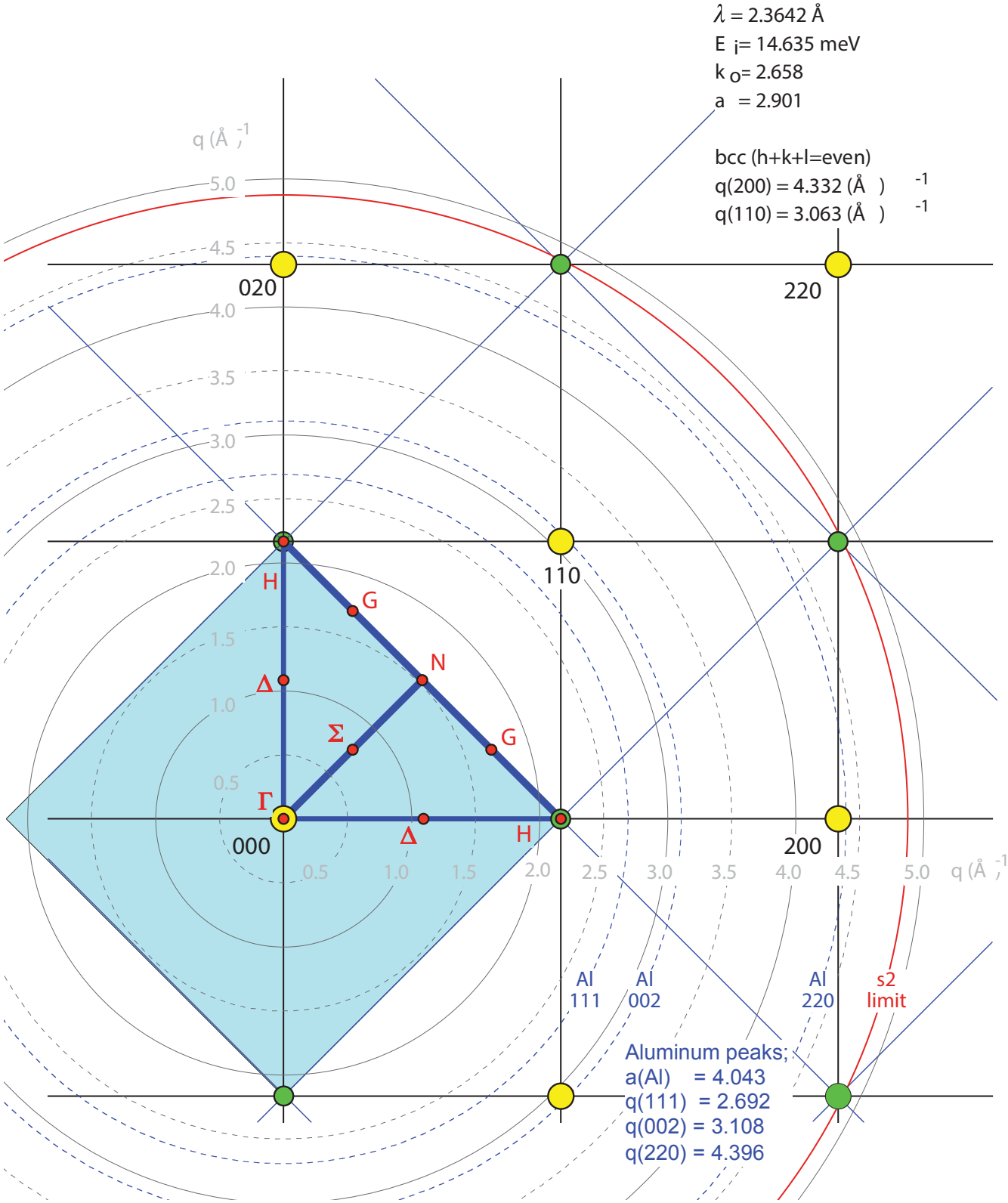
label	------- Site Occupancy -------		x	y	z	Num In Cell
Fe	Fe	1.000	0.0000	0.0000	0.0000	4
Fe	Fe	1.000	0.2500	0.2500	0.2500	8
Ga	Ga	1.000	0.5000	0.0000	0.0000	4
Ga	Ga	1.000	0.0000	0.5000	0.0000	4
Ga	Ga	1.000	0.0000	0.0000	0.5000	4

Total of: 24 atoms in the unit cell

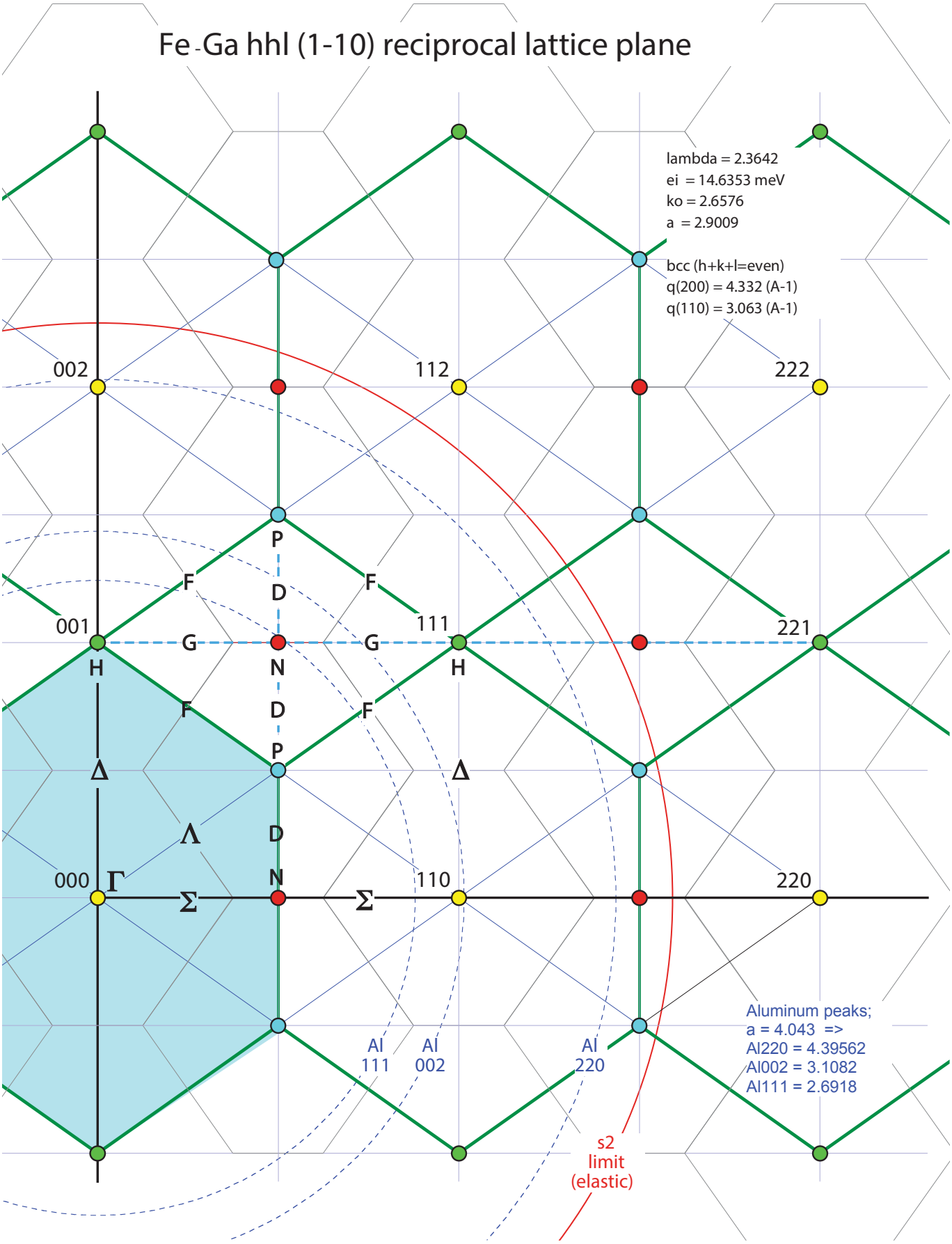
REFLECTIONS LIST
Neutron wavelength = 2.3560 A
Notes:
1. Intensities are relative to 1 cubic Angstrom of material
2. multiplicities may show unexpected values if two reflections
with different sets of Miller Indices have the same d-spacing.
In these cases, CrystalDiffract lists the SUM of the multiplicities
for all reflections with the same d-spacing

ref no.	(N)	h	k	l	d(hkl)	2-Theta	Intensity	I/Imax	m(hkl)
[1]	3	1	1	1	3.34863	41.1931	1.43007e+02	1.4	8
[2]	4	0	2	0	2.90000	47.9336	7.62298e+01	0.7	6
[3]	8	2	0	2	2.05061	70.1241	1.07208e+03	10.4	12
[4]	11	1	3	1	1.74877	84.6938	9.54260e+01	0.9	24
[5]	12	2	2	2	1.67432	89.4284	3.00713e+01	0.3	8
[6]	16	4	0	0	1.45000	108.6649	3.71806e+02	3.6	6
[7]	19	3	1	3	1.33061	124.5787	1.15107e+02	1.1	24
[8]	20	0	4	2	1.29692	130.5446	1.30796e+02	1.3	24
[9]	24	2	4	2	1.18392	168.5354	1.02933e+04	100.0	24

Fe-Ga hk0 (001) reciprocal lattice plane

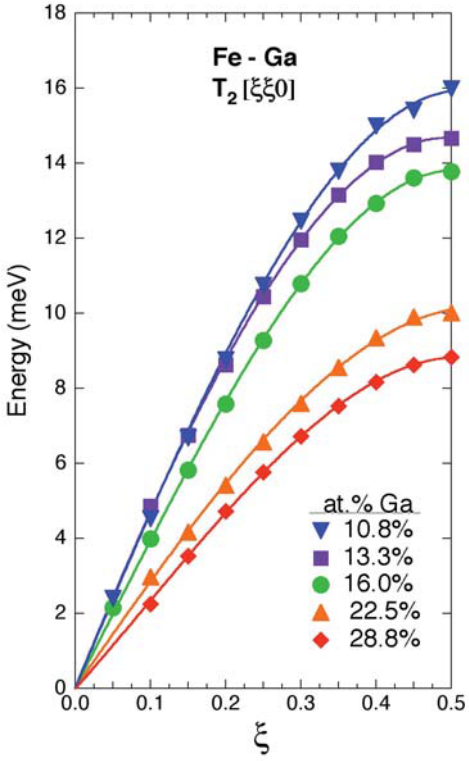


Fe-Ga hhl (1-10) reciprocal lattice plane

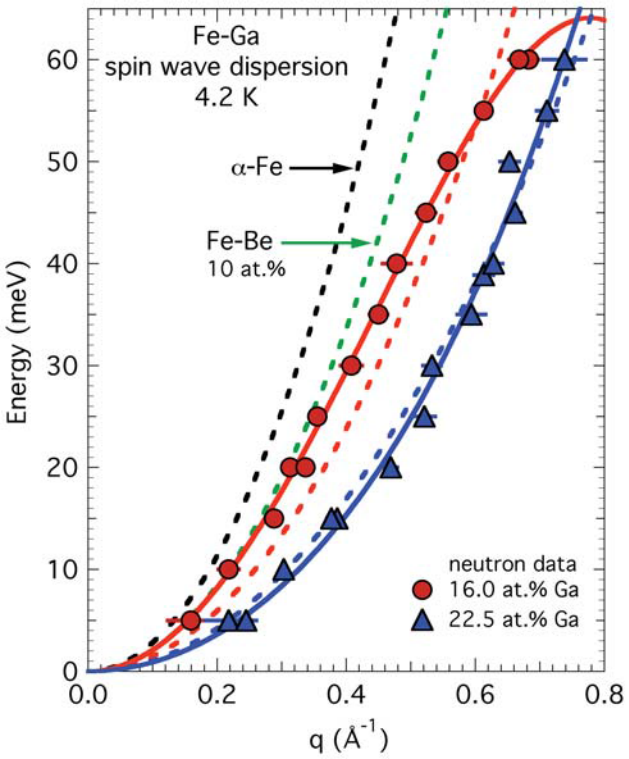


In the event of neutrons not being available for the neutron school, data sets for the Fe-Ga measurements can be found in the zipped file, “data.zip”. (note; the spin wave data in those files was taken in the hhl plane rather than the planned reciprocal lattice plane, hk0, for the neutron school experiments.

Phonon and spin wave dispersion curves are shown below.



T_2[110] phonon dispersion curves for five Fe-Ga compositions.



Measured spin wave dispersion of two Fe-Ga compositions with comparison to α-Fe and Fe-Be 10 at.%.

Fe-Ga lattice parameter vs. composition, phonon spin wave experimental data (found in zipped file, spin wave experiments were in the hhl plane);

		experiment #’s	
Ga at.%	a (Å)	phonons	spin waves
10.8	2.89	60	174
16.0	2.90	56	229
22.5	2.91	66	228
28.8	2.92	118	222

Example; Fe-Ga 28.8 at.% T2[100] phonon scans

After sample alignment and calibration scan check, the above phonon dispersion curves can be used to get the energy range for constant-Q phonon scans for your sample. Edit the focusing check scans for that energy (also modified for neutron energy loss at HB1 and HB3) to determine direction of q from the 110 reciprocal lattice point. Edit remaining T2 branch scans for correct focusing and energy range.

Edit the rest of the T2 branch scans for energy range required.

```
(count rate set to 1 mcu = ~1 sec)
comment "calibration scans Fe-Ga XX.X%, attenuated (?) beam"

scantitle "calibration (200) Trans"
scan h 2 k -0.05 0.05 0.005 l 0 e 0
scantitle "calibration (200) Long"
scan h 1.95 2.05 .005 k 0 l 0 e 0

scantitle "calibration (020) Trans"
scan h -0.05 0.05 0.005 k 2 l 0 e 0
scantitle "calibration (020) Long"
scan h 0 k 1.95 2.05 .005 l 0 e 0
```

focusing check scans (T2[110]) for HB1A at q = 0.1;

```
scantitle "T2[110] q = 0.1, focusing check, e-gain"
scan h 0.9 k 1.1 l 0 e -1 -7 -.25 preset mcu 10
comment “previous scan gives 1000 cts pkht / 50 cts bkg, @ 10 sec/pt”
scan h 1.1 k 0.9 l 0 e -1 -7 -.25 preset mcu 10
```

T2[110] branch (again HB1A, neutron energy gain!);

```
scantitle "T2[110] q = 0.05"
scan h 0.95 k 1.05 l 0 e -1 -7 -.20 preset mcu 10
comment “previous scan not successful at HB1A”
scantitle "T2[110] q = 0.15"
scan h 0.85 k 1.15 l 0 e -1 -7 -.25 preset mcu 10
scantitle "T2[110] q = 0.20"
scan h 0.80 k 1.20 l 0 e -1 -9 -.25 preset mcu 20
scantitle "T2[110] q = 0.30"
scan h 0.70 k 1.30 l 0 e -2 -11 -.4 preset mcu 40
scantitle "T2[110] q = 0.40"
scan h 0.60 k 1.40 l 0 e -3 -14 -.5 preset mcu 60
scantitle "T2[110] q = 0.50"
scan h 0.50 k 1.50 l 0 e -4 -16 -.5 preset mcu 60
comment “350 cts pkht over a bkg of 75 cts, @ 60 sec/pt”
```

Spin wave scans (constant energy transfer);

The low energy (T110 and L110 from the 110) scans (5 and 10 meV) should be good scans to show dispersion on both sides of the 110 r.l. pt. as well as picking up both spin waves and phonons in the same scan. These scans were on an Fe3Ga sample, the only sample I measured spin waves in the hk0 plane at HFIR. (All the Fe-Ga spin wave scans were in the hhl plane.) Again, scans are from HB1A so e-gain is used (except for the two noted at 5 meV).

Transverse and Longitudinal 110 scans from the 110;

```
scantitle "sw; T110 fr 110, 5 meV"
scan h .75 1.25 .01 k 1.25 .75 -.01 l 0 e -5 preset mcu 10
scantitle "sw; L110 fr 110, 5 meV"
scan h .75 1.25 .01 k .75 1.25 .01 l 0 e -5 preset mcu 10

scantitle "sw; T110 fr 110, 5 meV, e-loss"
scan h .75 1.25 .01 k 1.25 .75 -.01 l 0 e 5 preset mcu 10
scantitle "sw; L110 fr 110, 5 meV, e-loss"
scan h .75 1.25 .01 k .75 1.25 .01 l 0 e 5 preset mcu 10

scantitle "sw; T110 fr 110, 10 meV"
scan h .7 1.3 .01 k 1.3 .7 -.01 l 0 e -10 preset mcu 50
scantitle "sw; L110 fr 110, 10 meV"
scan h .7 1.3 .02 k .7 1.3 .02 l 0 e -10 preset mcu 50

scantitle "sw; T110 fr 110, 15 meV"
scan h .64 .98 .01 k 1.36 1.02 -.01 l 0 e -15 preset mcu 50
scantitle "sw; L110 fr 110, 15 meV"
scan h .64 .98 .01 k .64 .98 .01 l 0 e -15 preset mcu 50

scantitle "sw; T110 fr 110, 20 meV"
scan h .64 .98 .01 k 1.36 1.02 -.01 l 0 e -20 preset mcu 75
scantitle "sw; L110 fr 110, 20 meV"
scan h .64 .98 .02 k .64 .98 .02 l 0 e -20 preset mcu 75
```

Transverse and Longitudinal 010 scans from the 110;

```
scantitle "sw; T010 fr 110, 5 meV"
scan h 1 k 1.02 1.36 .02 l 0 e -10 preset mcu 10

scantitle "sw; T010 fr 110, 10 meV"
scan h 1 k 1.02 1.36 .02 l 0 e -10 preset mcu 40

scantitle "sw; T010 fr 110, 15 meV"
scan h 1 k 1.02 1.36 .02 l 0 e -15 preset mcu 60

scantitle "sw; T010 fr 110, 20 meV"
scan h 1 k 1.02 1.36 .02 l 0 e -20 preset mcu 75
```