EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

CERN-PPE/93-06
11.01.1993

LATTICE SITE AND HYPERFINE FIELD OF Fr IN Fe STUDIED BY NUCLEAR ORIENTATION AND EMISSION CHANNELLING

M. Lindroos[a)], P. Richards[b)], J. De Wachter[c)], U. Wahl[d)], H. Haase[e)], H. Pattyn[c)],. J. Rikovska[b)], N.J. Stone[b)], K. Nishimura[f)], I.S. Oliveira[b)], M. Veskovic[e)]

and the NICOLE and ISOLDE collaborations

ABSTRACT

The issue of lattice sites of Fr in Fe has been studied with two different techniques, integral Low Temperature Nuclear Orientation (LTNO) and emission channelling. Monte Carlo simulations of the system fitted to the channelling spectra reveal a large fraction of Fr in substitutional sites and hint at a possible complex site distribution. Using a two site model for the LTNO data, a large fraction in high field site, in agreement with the channelling data, is deduced.

(IS01-23)

Presented at the IXth International Conference on Hyperfine Interactions,Toyonaka, Osaka, Japan, 17-21 August 1992
To be published in Hyperfine Interactions

---

a) Physics Dept., Chalmers Univ. of Technology, Gothenburg, Sweden
b) Physics Dept., Oxford University, Oxford, UK
c) Inst. voor Kern- en Stralingsfysika, KU Leuven, Leuven Belgium
d) Fakultät für Physik, Universität Konstanz, Konstanz, Germany
e) ISOLDE, CERN, Geneva, Switzerland
f) Physics Department, Toyama University, Toyama, Japan

LATTICE SITE AND HYPERFINE FIELD OF Fr IN Fe STUDIED BY NUCLEAR ORIENTATION AND EMISSION CHANNELLING

M.Lindroos[a], P.Richards[b] J.De Wachter[c], U.Wahl[d] H.Haase[e], H.Pattyn[c], J.Rikovska[b], N.J.Stone[b], G.Langouche[c], K.Nishimura[f], I.S.Oliveira[b] and M.Veskovic[e], the NICOLE and ISOLDE collaborations

a Physics Dept, Chalmers Univ. of Technology, Gothenburg, Sweden
b Physics Dept., Oxford University, Oxford, UK
c Inst. voor Kern- en Stralingsfysika, KU Leuven, Leuven, Belgium
d Fakultät für Physik, Universität Konstanz, Konstanz, Germany
e ISOLDE, CERN, Geneva, Switzerland
f Physics Dept, Toyama University, Toyama, Japan

The issue of lattice sites of Fr in Fe has been studied with two diffrent techniques, integral Low Temperature Nuclear Orientation (LTNO) and emission channelling. Monte Carlo simulations of the system fitted to the channelling spectra reveal a large fraction of Fr in substitutional sites and hint at a possible complex site distribution. Using a two site model for the LTNO data, a large fraction in high field site, in agreement with the channelling data, is deduced.

1.Introduction

A question of fundamental interest for our understanding of the technologically important implantation process into solids is the final lattice site of the primary ions. This work will discuss the lattice site of francium studied by two different methods, emission channelling and integral LTNO.

Fr in Fe has been studied by integral On-Line LTNO earlier by J.Wouters et al [1]. Using a two-site model they deduced a high fraction, f_s=78(3)% with a hyperfine field B_{hf}=70(5) T, of Fr in large field sites at a total dose of nominally 10^{12} atoms cm^{-2}. A systematic RBS channelling study by O.Meyer and A.Turos [2] revealed zero substitutional fraction for the next lighter alkali element Cs at a total dose of 10^{13} atoms cm^{-2}. Meyer et al proposed a model relating the enthalpy of solution as defined by

Miedema [3] to the substitutional fraction. According to this model zero substitutionality for Fr, which has a even larger enthalpy of solution than Cs, is expected. However, models based on kinematic arguments [4,5] do predict considerable fraction in substitutional sites even for these large ions.

Integral LTNO studies give an average value for the hyperfine field of all those atoms in lattice positions with a large enough field to give appreciable polarisation of the nucleus. The hyperfine field for individual lattice sites in an unknown distribution can not be deduced. Therefore it is important to do complementary experiments. In the technique of NO this can be done with a resonance experiment, NMR-ON, but it has proved difficult to resonate all sites [6]. An alternative method is the use of channelling. We have performed an emission channelling experiment on Fr in Fe revealing a high fraction in substitutional site in agreement with the LTNO experiment.

2. Experiments

For the LTNO experiment the source was prepared at the ISOLDE-2 separator, CERN, by implantation at 60 keV of the ^{225} Ra isotope into a Fe foil at room temperature. The 99.999% pure Fe foil was rolled and polished to a thickness of 0.1 mm. The total implant dose was approximately $2x10^{13}$ ions over an area of 0.3 cm^2.The decay chain of ^{225}Ra can be seen in figure 1. The typical alpha decay energy is 7 MeV giving a nuclear recoil energy of approximately 130 keV which is sufficient for re-implanting the recoiling nucleus. Thus each member of the decay chain is re-implanted at low-temperature during the measurement. The recoil energy is high enough to eject some of the nuclei from the foil, a fact that has to be taken into consideration in determining the fraction in high field sites in the analysis. Two different anisotropy experiments were made on the source, a gamma emission and an alpha particle experiment [7].

The emission channelling experiment was performed on-line at the ISOLDE-2 facility. The ion-beam was collimated to a

diameter of 150 μm and implanted at a geometry permitting simultaneous measurement with a position sensitive silicon detector (see figure 2). Two isotopes of Fr were studied; the shortlived ^{213}Fr isotope, $T_{1/2}$=34.6 s, and the longer lived ^{221}Fr isotope, $T_{1/2}$=4.9 min. The experiment was performed at two temperatures; room temperature and 120 K. The silicon detector gives both position and energy signals thus allowing separation of the channelling patterns from different members of the decay chain through gating in the energy spectrum. The experiment was performed with an average flux of 1.8 x 10^5 francium ions per second resulting in a maximum dose well below 10^{12} cm^{-2}. [8].

3. Analysis and results

From the gamma emission experiment using a two-site model an upper and lower limit for the fraction in good sites can be extracted, 38% < f < 45% [7]. Taking the known value for μ (μ=+1.58(3) nm [9]), the fitted value for μB_{hf} product gives B_{hf}(Fr<u>Fe</u>)= (+) 129.7(40) . The fitted value for μB_{hf} in the alpha emission experiment, B_{hf}(Fr<u>Fe</u>)= (+) 141.1(95) is within error limits in agreement with the gamma emission anisotropy results, see figure 3.

The emission channelling data have been been analyzed using a channelling simulation code. The program is developed by P.J.Smulders and D.O.Borma [10]. It combines the binary collision model and the multistring approximation and produces simulated scans which can be fitted to the experimental data. In our analysis we fitted the following free parameters: lattice site (random site, substitutional site, octahedral site and tetrahedral site) and vibration amplitude or static displacement of the francium atom. For iron an appropriate value for the vibration amplitude can be extracted from the Debye temperature, T_D(Fe)=470 K. For the Fr impurity the Debye temperature was taken to be T_D=236 K for the fits where the amplitude was a fixed parameter. The results from the different fits are presented in table 1 and the best fit, with random fraction, substitutional fraction and vibration amplitude or static displacement as free parameters is shown in figure 4. The

best fit results in a substitutional fraction of f_s=44(9)% and a vibration amplitude u_1=0.090(15) Å at room temperature. The results at 120 K are compatible with a vibration amplitude in the range 0.04 - 0.10 Å and a subtitutional fraction f_s=67(13)%. The result from the larger amount of data collected at room temperature shows that it is not impossible that up to 30% of the atoms can be in either tetrahedral or octrahedral sites.

4. Discussion

A considerable fraction of Fr in Fe is found in substitutional sites in the whole temperature range investigated. Kinematic models [5] predict 45(5)% in substitutional sites which is in good agreement with experimental results. The discrepancy between our results and O.Mayer and A.Turos systematics, where zero substitutionality was expected, could possibly be explained by a dose and temperature dependence[8].

Large vibration amplitudes of the studied impurity can be inferred from the narrowing of the blocking dips. However, the calculated widths of the blocking dips are sensitive to the model input parameters; i) Implantation profile depth, ii) angular resolution and iii) vibration amplitude of the host. A narrowing can also be caused by an amorphous layer on top of the crystal. However, these parameters can only account for up to a 10% narrowing of the dips which is a factor of two smaller than observed. Therefore, we can conclude that the large deduced vibration amplitude is a true phyics effect which can be interpreted as either a vibration or a static displacement of the Fr atom. We imagine it as a dislocation of 1/23 of a lattice constant connected to the trapping of single vacancies. Assuming similar implantation properties for Cs in Fe, the large displacements could explain the very broad NMR-ON resonance observed by Ashworth et al [6].

The observed dose and temperature dependence of the lattice site distribution is most likely the cause of the discrepancy

between the integral LTNO hyperfine field B_{hf}=129.7(40) T in our experiment and B_{hf}=70(5) T in the experiment by J.Wouters et al [1]. Our LTNO experiment was carried out at an initially higher implantation dose of the mother nucleus ^{225}Ra. However, the local dose of Fr during the measurement was very low. The sample was left at room temperature between measurements sufficiently long time for primary damage to anneal out. The pattern from the case of Cs in Fe [6] is then repeated, the low dose implant at low temperature gives a high field site. In the Wouters experiment which was fully on-line there was no opportunity for annealing of primary damage. Furthermore, the implant dose on-line is often higher than measured from the activity as a result of other ions being present in the beam.

References

[1] J.Wouters, N. Severijns, J. Vanhaverbecke, W Vanderpoorten and L.Vanneste, Hyp.Int. 61 (1990) 1391

[2] O.Meyer and A.Turos, Mater.Sci.Rep. 2 (1987) 371

[3] A.R.Miedema, P.F.Châtel and F.R. de Boer, Physica B, 100 (1980) 1

[4] C.Erginsoy, G.H.Vineyard and A.Englert, Phys.Rev.A, 133 (1964) 595

[5] D.K.Brice in: Applications of Ion Beams to Materials 1975, eds G.Carter, J.S.Colligon and W.A.Grant (Inst. of Phys., London 1976) no.28, p.334

[6] C.J.Asworth, P.Back, S.Ohya, N.J.Stone and J.P.White, Hyp.Int. 59 (1990) 461

[7] M.Lindroos, P.Richards, J.Rikovska, N.J.Stone, I.Oliveira, K.Nishimura, M.Booth and the NICOLE and ISOLDE collaborations, Accepted for publication in Hyp.Int.

[8] M.Lindroos, H.Haas, J.De Wachter, H.Pattyn and G.Langouche, Nuclear Instr. and Methods B 64 (1992) 256

[9] P.Raghavan, Atom. Nucl. Data Tables 42 (1989) 189.

[10] P.J.M.Smulders and D.O.Boerma, Nuclear Instr. and Methods B 29 (1987) 471

Figure Captions

Figure 1. Simplified decay scheme of ^{225}Ra

Figure 2. Two dimensional plot in the <111> direction. The blocking dip and the blocking patterns are clearly visible.

Figure 3. Temperature dependence of the 6.24 MeV alpha transition and the 217 KeV gamma transition from ^{221}Fr. Full line shows adopted best fit; B_{hf}=129.7(40) T and 38%<f<45% for the gamma emission experiment and B_{hf}=141.1(95) T for the alpha particle experiment. Dotted line shows best fit assuming B_{hf}=70 T.

Figure 4. The best fit for the simulated channelling spectra to all the experimental data. Free parameters in the fit were fraction in subtitutional site, random fraction and vibration amplitude. The fit results in f_s=44(9)%, f_R=66% and u_1=0.090(15) Å at room temperature and f_s=67(13)%, f_R=33% and u_1=0.10 Å at 120 K.

Table captions

Table1. Result of the fit for the simulated channelling spectra to the emission channelling data. Parameters with a F were kept fixed with given value in the fitting procedure. The total count rate in the data taken at 120 K was not sufficient to permit a fit of more than three free parameters.

Temp	Direction	f_R	f_S	f_O	u_1	χ^2_r
300 K	<100>	0.63	0.37	0 F	0.061 F	0.89
300 K	<110>	0.55	0.45	0 F	0.061 F	1.32
300 K	<111>	0.68	0.32	0 F	0.061 F	1.17
120 K	<100>	0.60	0.40	0 F	0.040 F	0.94
120 K	<110>	0.32	0.68	0 F	0.040 F	0.90
120 K	<111>	0.51	0.49	0 F	0.040 F	0.91
300 K	<100>	0.61	0.39	0 F	0.08	0.82
300 K	<110>	0.44	0.57	0 F	0.10	1.04
300 K	<111>	0.64	0.36	0 F	0.09	0.98
120 K	<100>	0.47	0.53	0 F	0.10	0.92
120 K	<110>	0.16	0.84	0 F	0.10	0.89
120 K	<111>	0.38	0.62	0 F	0.11	0.90
300 K	<100>	0.39	0.26	0.35	0.061 F	0.82
300 K	<110>	0.31	0.37	0.32	0.061 F	1.44
300 K	<111>	0.32	0.35	0.32	0.061 F	1.32
300 K	<100>	0.37	0.28	0.35	0.08	0.86
300 K	<110>	0.19	0.52	0.29	0.10	1.09
300 K	<111>	0.31	0.39	0.30	0.09	1.00

Table I

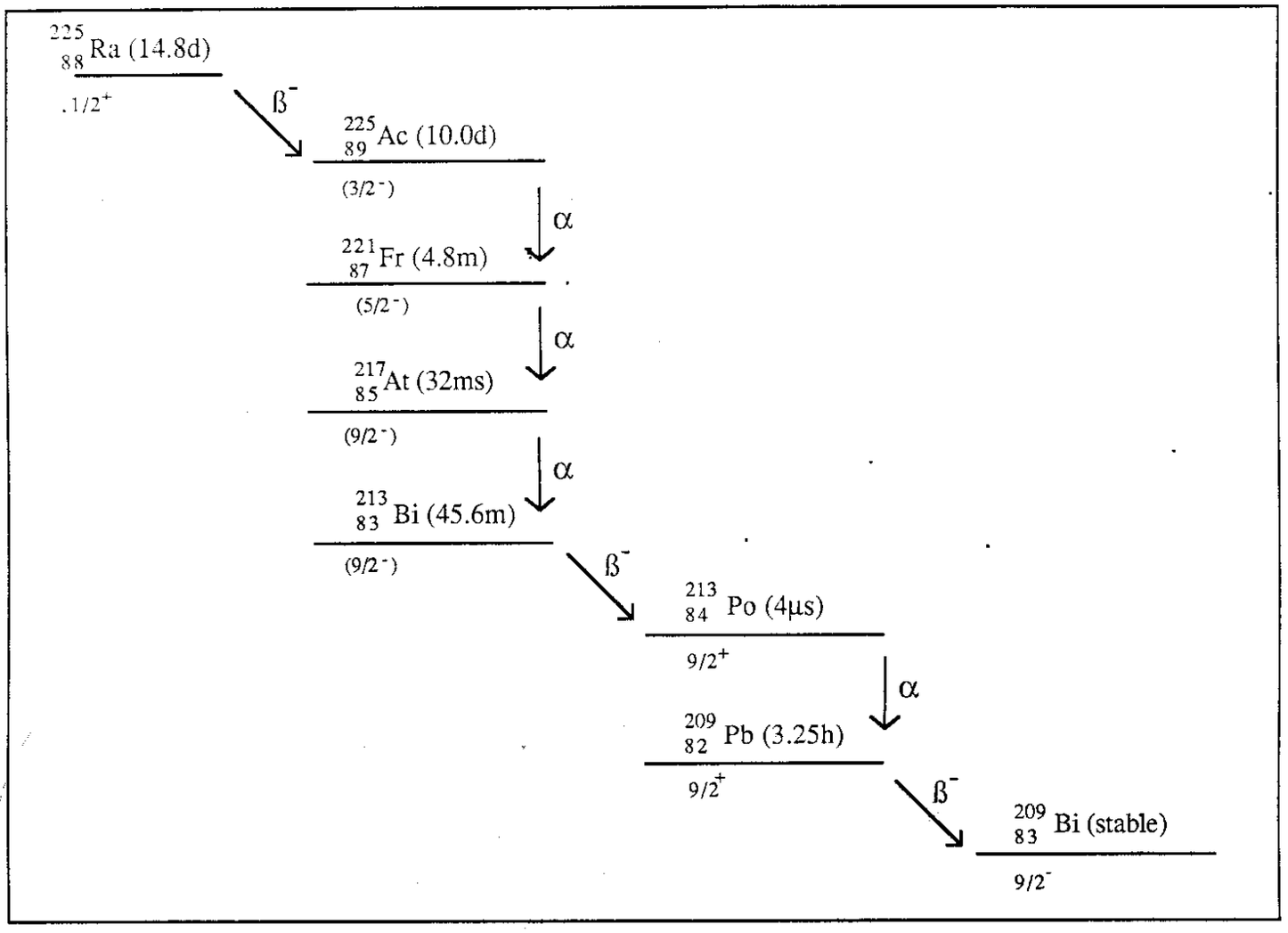
225 88 Ra (14.8d)
.1/2+
ß-
225 89 Ac (10.0d)
(3/2-)
α
221 87 Fr (4.8m)
(5/2-)
α
217 85 At (32ms)
(9/2-)
α
213 83 Bi (45.6m)
(9/2-)
ß-
213 84 Po (4µs)
9/2+
α
209 82 Pb (3.25h)
9/2+
ß-
209 83 Bi (stable)
9/2-

Fig. 1

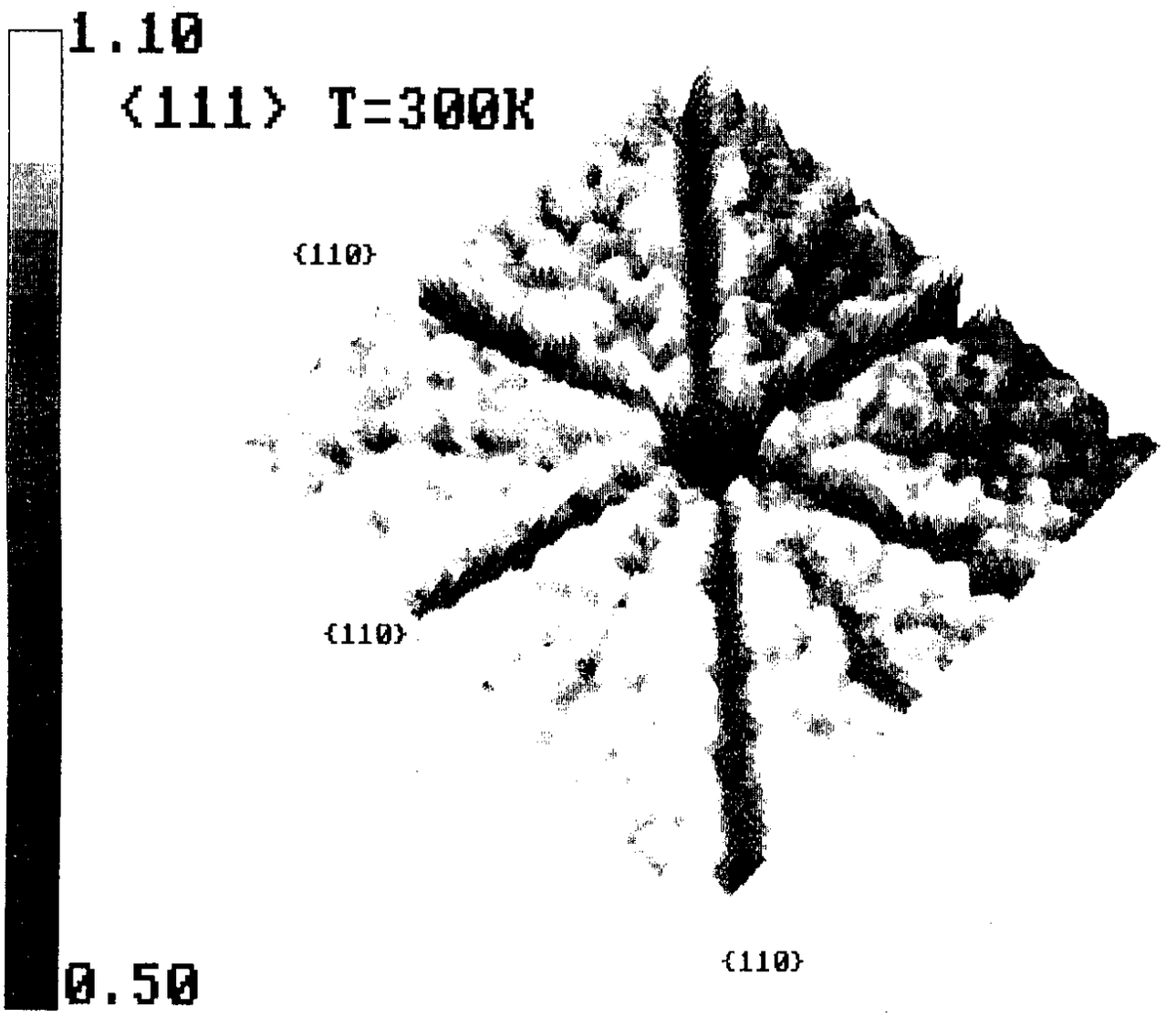

Fig. 2

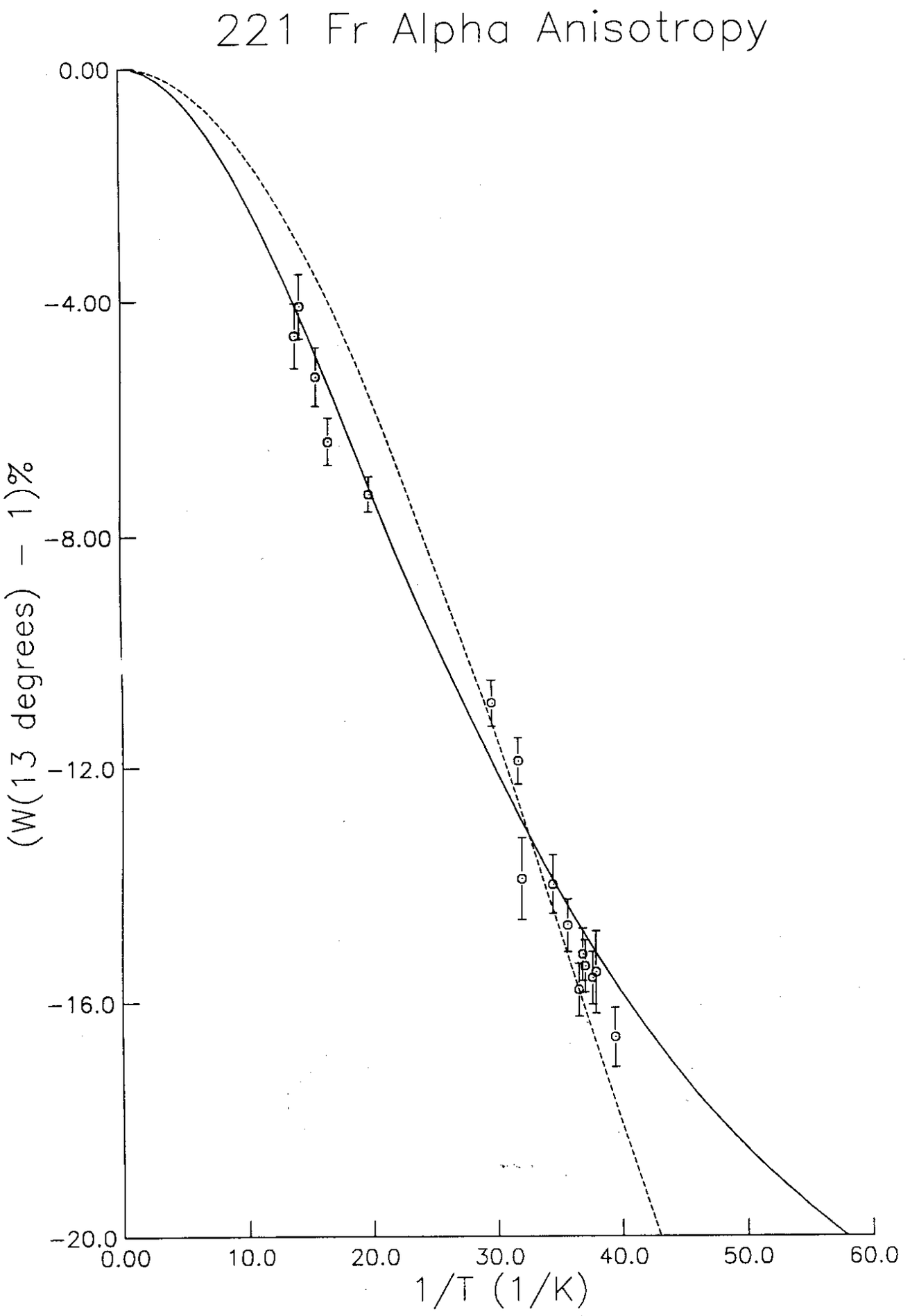
221 Fr Alpha Anisotropy
0.00
-4.00
-8.00
-12.0
-16.0
-20.0
(W(13 degrees) - 1)%
0.00
10.0
20.0
30.0
40.0
50.0
60.0
1/T (1/K)

Fig. 3

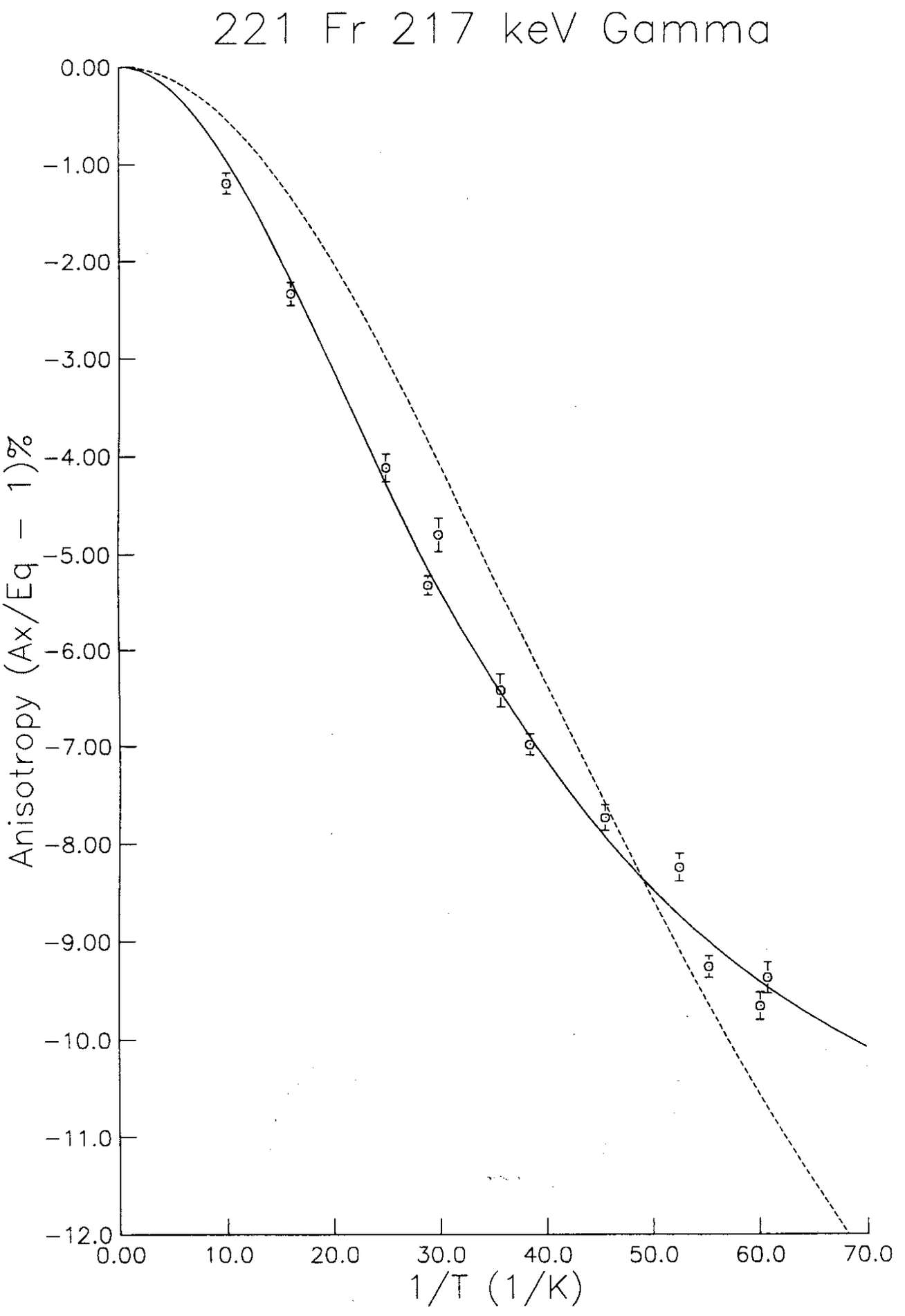
221 Fr 217 keV Gamma
Anisotropy (Ax/Eq - 1)%
0.00
-1.00
-2.00
-3.00
-4.00
-5.00
-6.00
-7.00
-8.00
-9.00
-10.0
-11.0
-12.0
0.00
10.0
20.0
30.0
40.0
50.0
60.0
70.0
1/T (1/K)

Fig. 3 bis

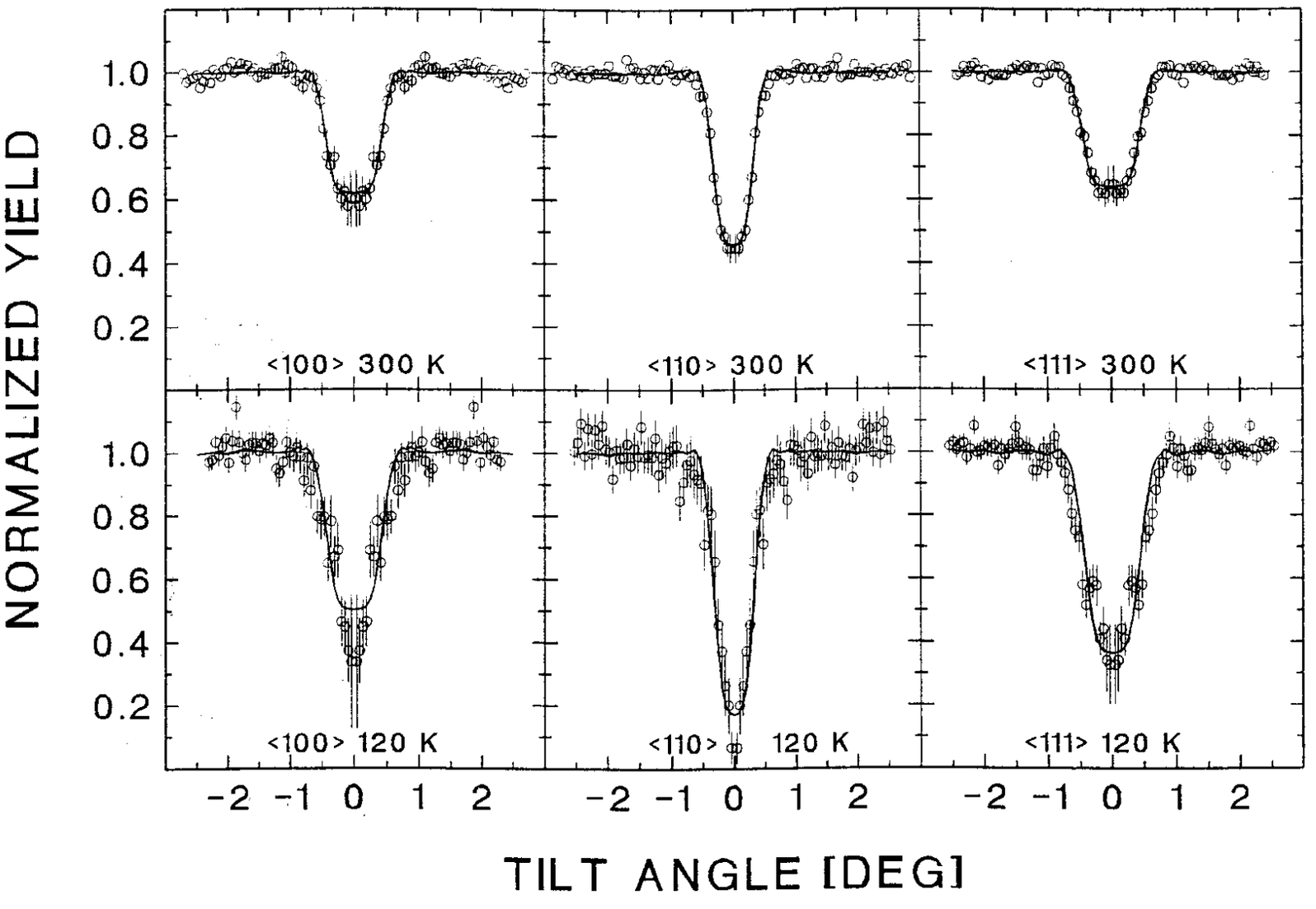
NORMALIZED YIELD
1.0
0.8
0.6
0.4
0.2
<100> 300 K
<110> 300 K
<111> 300 K
<100> 120 K
<110> 120 K
<111> 120 K
-2 -1 0 1 2
TILT ANGLE [DEG]

Fig. 4