УДК 537.621
doi: 10.18101/ 978-5-9793-0898-2-162-168

COMPARING CALCULATION OF X-RAY AND NEUTRON DIFFRACTION INTENSITIES FOR $Nd_2Fe_{14}B$

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Time-of-Flight (TOF) neutron diffraction experiment carried out on hard magnetic material $Nd_2Fe_{14}B$ at the High-Resolution Fourier Diffractometer (HRFD) of Frank Laboratory of Neutron Physics, Joint Institute for Nuclear research (JINR), Dubna, Russia. The atomic and structure factors, intensities of neutron diffraction reflections for crystal $Nd_2Fe_{14}B$ have calculated MathLab program. A numerical results compared with neutron diffraction experimental data and calculation for X-Ray diffraction reflections .
Keywords: $Nd_2Fe_{14}B$, neutron diffraction, x-ray diffraction, atomic factor, structure factor.

Introduction

The Nd-Fe-B permanent magnet is the strongest magnet in the world. The magnetic power of Rare Earth Element (REE) system magnets increases rapidly, for instance, from Sm-Co system to Nd-Fe-B system. There are many applications in the various field.

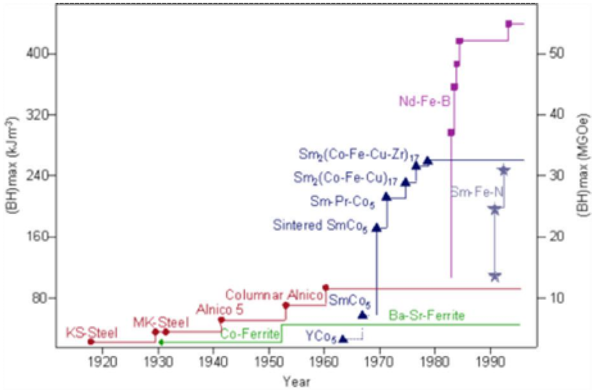

Fig. 1. History of permanent magnets

Especially, Generator and motor for Hybrid cars is operated at high temperature, for instance, $200C^0$ Figure1. and Figure2. shows the history and the applications of permanent magnets [1].

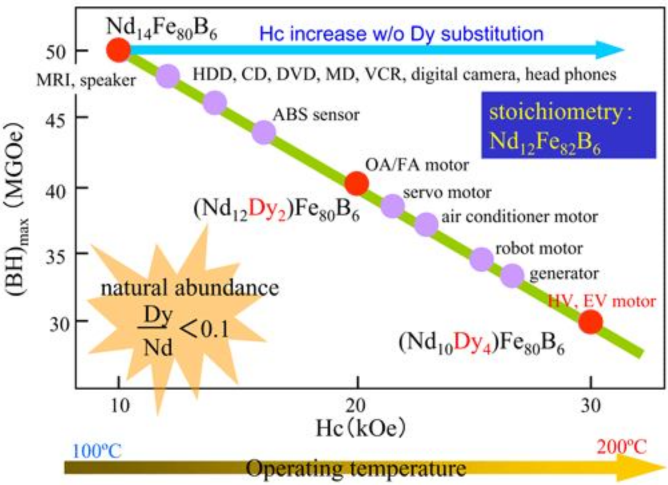

Fig. 2. Application of NdFeB magnets

Experimental

The diffraction patterns were measured with HRFD instrument at the IBR-2 pulsed reactor high resolution Furrier-diffractometer of Frank Laboratory of Neutron Physics, JINR, Dubna, Russia. At this diffractometer the correlation technique of data acquisition is used, which provides a very high resolution (Δd/d ≈ 0.0013) that is practically constant in a wide interval of dhkl spacing's at HRFD (Figure3) diffraction patterns are measured at fixed scattering angles 2θ = ±152° in the wavelength range of 1 — 8 Å.

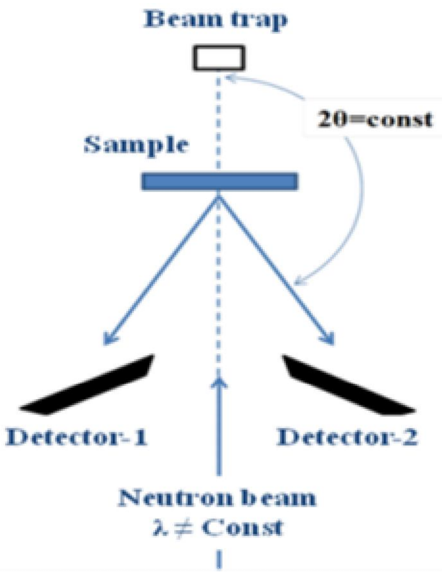

Fig. 3. The principal plan of HRFD

One of the most important feature of neutron diffraction is a high penetration length (~1 cm), which helps investigating bulky materials [2]. A part of Neutron diffraction of $Nd_2Fe_{14}B$ (Figure 4).

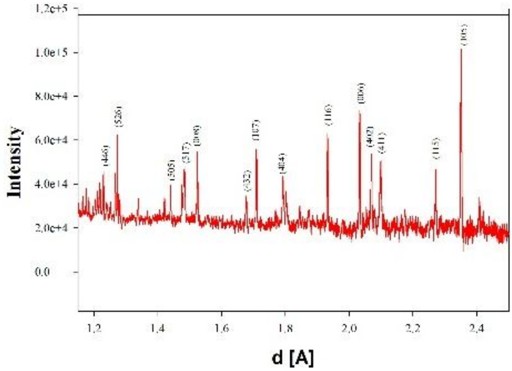

Fig. 4. Neutron diffraction pattern for $Nd_2Fe_{14}B$ after normalization at T=473K

Crystal structure

The $Nd_2Fe_{14}B$ have tetragonal crystal structure unit cell parameter a=b=8.80Å, c=12.19Å, α=β=γ=90°and their symmetry space group is $P4_2/mnn$ (No.136)[3].

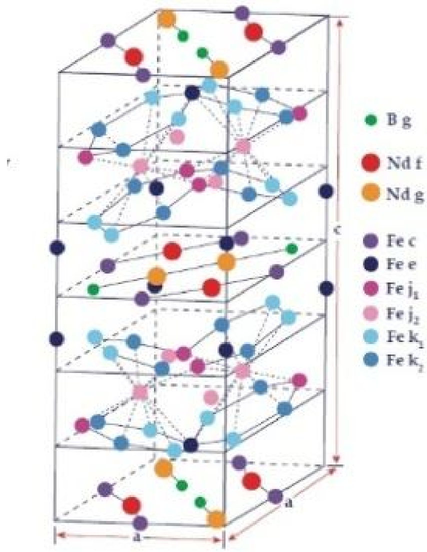

Fig. 5. The neutron diffraction of $Nd_2Fe_{14}B$

Intensity of X-ray diffraction of $Nd_2Fe_{14}B$ crystal depends on structure factor which depends upon positions of atoms and Miller index (hkl) of planeand atomic scattering factor $f_j$from value of diffraction angle[4].

$$F_{hkl}^{XRD} = \sum_{j=1}^{N} f_j e^{[2\pi i(hx_j+kh_j+lz_j)]} \quad (1)$$

Here, hkl –Miller index, x_j, y_j, z_j-atomiccoordinates,f_j- atomic scattering factor.

In general, atomic scattering factor for x-ray is [3]:

$$f \; = a_0 + a_1\left(\frac{sin\theta}{\lambda}\right) + a_2\left(\frac{sin\theta}{\lambda}\right)^2 + \cdots a_7 \quad (2)$$

Intensity of neutron diffraction of the crystal depends heavily on structure factor which depends upon positions of atoms in Miller index (hkl) planeand atomic scattering length $b_j$which is not dependent from diffraction angle[2].

$$F_{hkl}^{ND} = \sum_{j=1}^{N} b_j e^{[2\pi i(hx_j+kh_j+lz_j)]} \quad (3)$$

Calculation of atomic and structure factor

We have calculated atomic factors and structure factors of X-ray diffraction peak intensities of $Nd_2Fe_{14}B$ crystal using equations (1), (2) and values from Table.1 by using MATLAB program. Results are shown in Table.2

Table 1

Atomic Site Occupancies and Coordinates$Nd_2Fe_{14}B$

Atom	Site	Occ	Ze	x	Y	z	bj
d	F	4	60.60	0.266	0.266	0	7.7
Nd	G	4	60.60	0.139	-0.14	0	7.7
Fe	k1	16	26.26	0.224	0.568	0.128	9.45
Fe	k2	16	26.26	0.039	0.359	0.176	9.45
Fe	j1	8	26.26	0.097	0.097	0.205	9.45
Fe	j2	8	26.26	0.318	0.318	0.247	9.45

Fe	E	4	26.26	0.5	0.5	0.113	9.45
Fe	C	4	26.26	0	0.5	0	9.45
B	G	4	5.50	0.368	-0.37	0	5.3

Here: Ze-atomic number, x,y,z-atomic coordinate, bj-atomic scattering length

Table 2

.$Nd_2Fe_{14}B$atomic factor, structure factor of values

(hkl)	**d_{hkl}**	**mult**	**F-cal**	**I-experiment**
(015)	2.35	8	18.75	43.35
(040)	2.23	8	3.08	46.35
(140)	2.13	8	52.64	70.01
(141)	2.1	16	100	100
(042)	2.07	8	2.91	52.09
(006)	2.03	2	0.3	42.77
(116)	1.93	8	5.31	60.6
(044)	1.79	8	12.6	55.04
(017)	1.71	8	14.39	61.6
(245)	1.53	2	1.82	37.51
(346)	1.33	16	12.09	46.4
(256)	1.27	16	6.11	37.2
(148)	1.24	8	5.45	43.07

(hkl)	**d_{hkl}**	**2θ**	**Int**	**Sinθ/λ**	**f_i**	**F-cal**
(105)	2.35	38.26	50.86	0.21	48.21	49.73
(115)	2.23	39.66	1.70	0.22	48.21	1.78
(410)	2.13	42.32	100	0.23	19.37	100
(411)	2.1	43	63.57	0.24	19.37	53.51
(402)	2.07	43.72	11	0.24	19.37	1.45
(006)	2.03	44.54	18.67	0.25	19.37	41.03
(116)	1.93	46.99	8.56	0.26	19.37	3.53
(404)	1.79	51.17	3.78	0.28	19.37	4.97
(107)	1.71	53.58	1.79	0.29	2.62	61.54
(008)	1.53	60.70	6.76	0.33	6.88	51.90
(621)	1.32	67.8	4.15	0.36	6.88	53.13
(526)	1.27	74.44	1.02	0.39	6.88	2.61
(446)	1.23	77.16	1.29	0.40	6.88	41.24

Here: (hkl)-Miller index, d_{hkl}-d spacing, 2θ- diffraction angle, Sinθ/λ –specific value , f_i-atomic scaterring factor, F-structure factor,

We have calculated atomic scattering length and structure factors of neutron diffraction of $Nd_2Fe_{14}B$ crystal using equation (3) and values from Table.1 by MATLAB program. Results are shown in Table3.

Table 3. Neutron diffraction of $Nd_2Fe_{14}B$ crystal structure of structure factor and atomic scattering length of values.

Conclusion

We have successfully implemented neutron diffraction experiment on $Nd_2Fe_{14}B$ crystal structure at high resolution Furrier-diffractometer of Frank Laboratory of Neutron Physics, JINR, Dubna, Russia and by using the data, we have calculated the intensity of neutron diffractions , atomic factors, atomic scattering length and structure factors at both x-ray and neutron diffraction conditions.

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СРАВНИТЕЛЬНОЕ ИССЛЕДОВАНИЕ МАГНЕТИКА $Nd_2Fe_{14}B$
С ПОМОЩЬЮ РЕНТГЕНОВСКОЙ И НЕЙТРОННОЙ ДИФРАКЦИИ

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Проведен нейтронографический эксперимент на сильном магнетике $Nd_2Fe_{14}B$ с помощью Фурье дифрактометра из Лаборатории нейтронной физики Объединенного института ядерных исследований с высокой разрешающей способностью, Дубна, Россия. Атомные и структурные факторы, интенсивности нейтронных дифракционных отражений для кристалла $Nd_2Fe_{14}B$ рассчитаны с помощью программы MathLab. Проведено сравнение численных результатов с нейтронографическими и рентгенографическими экспериментальными данными.

Ключевые слова: $Nd_2Fe_{14}B$, дифракции рентгеновских и нейтронных лучей, атомный фактор, структурный фактор.