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## **ЭНЕРГИЯ КУЛОНОВСКОГО ВЗАИМОДЕЙСТВИЯ В МДП СТРУКТУРЕ С ТОНКИМ ОКСИДНЫМ СЛОЕМ**

В инверсионном канале МДП структуры обсуждены свойства потенциала кулоновского взаимодействия с учетом конечности толщины диэлектрического слоя и диэлектрической неоднородности среды. В частности, получен явный вид зависимости кулоновского потенциала взаимодействия от толщины оксидного слоя. Показано, что кулоновское взаимодействие проявляется более эффективно в МДП структуре на базе  $\text{InSb/SiO}_2$ .

**Ключевые слова:** инверсионный канал, потенциал взаимодействия, высокий (низкий) -  $\kappa$  диэлектрический контраст.

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## **CHARACTERIZING THE LATTICE PARAMETERS IN IRON-DOPED LITHIUM NIOBATE CRYSTALS WITH DIFFERENT STOICHIOMETRY**

Lattice parameters  $a$  and  $c$  have been investigated for iron-doped lithium niobate crystals with different stoichiometry by using powder X-ray diffraction. The results were compared with the ones obtained for pure lithium niobate crystals.

**Keywords:** X-ray diffraction, lithium niobate, lattice parameters.

### **1. Introduction**

Lithium niobate crystal is one of the important synthetic crystals which is an attractive material for digital holographic memory storage due to its good photorefractive properties [1]. For the first time, light induced refractive index variation, the so-called photorefractive effect was investigated in 1966 by Ashkin et al. [2] utilized by Chen et al. [3] for the storage of volume phase holograms. The improvement of the photorefractive performance of lithium niobate is controlled by doping with transition metal ions, non photorefractive ions and by crystal composition as photorefractivity depends on the crystal structure and the content of intrinsic defects [4]. Among them, Fe-doped LN crystal is the most suitable material for data storage as it provides high capacity, rapidly transfer rate, good sensitivity and long data retention time.

The first investigation of the lithium niobate crystal structure was performed by Abrahams et al. [5]. Later studies of the lattice structure by X-ray and neutron

diffraction of single crystals or powder emphasized a decrease in the lattice parameters  $a$  and  $c$  with the increase of stoichiometry [6-9]. Recently, the dependence of the lattice parameters on the introduction of dopant ions [10, 11] was also shown.

A systematic study, including the influences of intrinsic defects and the introduction of Fe iron was not performed, thus the main intention of our investigation by means of X-ray powder diffraction reveals the dependence of the lattice parameters on these two factors.

## **2. The details of the experiment**

Sample preparation: Iron-doped lithium niobate crystals had been grown by the Czochralski technique from melts with different compositions:  $C_{Li}=48.2$ ;  $C_{Li}=48.45$ ;  $C_{Li}=50$ ;  $C_{Li}=54.5$  with a fixed dopant concentration (0.06 wt %) were expressed as S1, S2, S3, S4 respectively. The Li content in the crystal was determined by Raman backscattering spectroscopy [12]. The measurements have been performed in the Y(ZZ)Y backscattering configuration for all samples by using the LabRAM HR Evolution spectrometer in order to obtain the  $A_1TO$  modes.

For X-ray diffraction analysis the powder samples from the above mentioned crystals have been used. The lattice parameter measurements have been performed with the help of Philips MRD (Material Research Diffractometer) diffractometer by utilizing Cu  $K\alpha$  radiation with wavelength  $\lambda=0.1540598$  nm and operating in the reflection configuration with Bragg–Brentano geometry.

A diffraction pattern plotting the intensities and the positions of the diffracted peaks of radiation against the angular  $2\theta$  position of the detector produces a diffractogram which typically contains many distinct peaks, each corresponding to a different interplanar spacing. In a diffraction pattern, the peak positions determine the interatomic distances. This is shown in Fig.1.

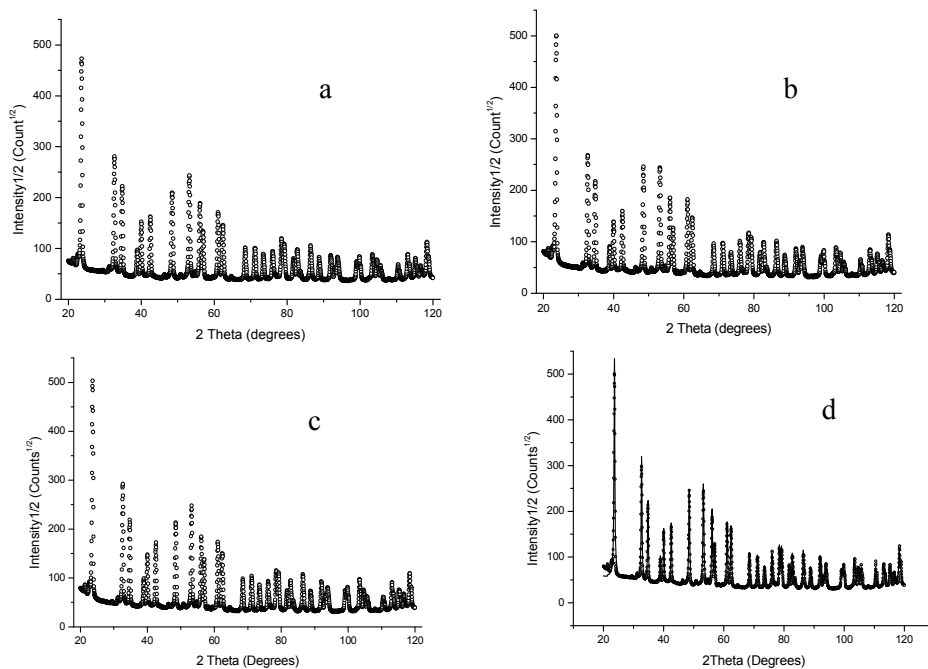


Fig. 1. a, b, c, -The XRD spectrum of  $2\theta$  (Intensity) for S1, S2, S3, S4 samples respectively, d- The result of the comparison of the XRD spectra for the S4 sample and the reference for the pure LN crystal

### 3. Results

In order to analyze the X-ray spectrum to obtain the lattice parameters a and c the peak positions were observed, comparing the experimental diffractograms with the calculated spectrum from the ICDD "Inorganic Crystal Structure Database" with the help of Maud (Materials Analysis Using Diffraction) computer program resulting in the automatic determination of the lattice parameters together with the instrumental parameters. In order to analyze the X-ray spectrum to obtain lattice parameters, the peak positions were observed, comparing the experimental diffractograms with the calculated spectrum from the ICDD "Inorganic Crystal Structure Database" with the help of Maud (Materials Analysis Using Diffraction) computer program resulting in the automatic determination of the lattice parameters together with the instrumental parameters. The diffractograms of the lithium niobate samples S1, S2, S3 are given in Fig. 1a-1c. The comparison of the experimental spectrum of the S4 sample with the computed one for the pure LN crystal from the ICDD is shown in Fig. 1d.

The obtained values of the lattice parameters for all samples under study are shown in Fig. 2 (depending on the composition of lithium niobate in the melt) compared with the ones known from literature [6-9] and Table.

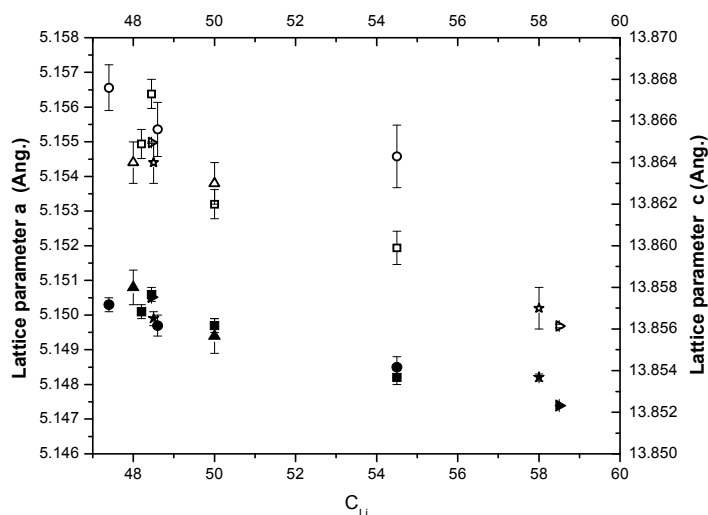


Fig. 2. The dependence of lattice parameters on the lithium niobate composition in the melt. Lattice parameter a: ■-our results, ▲-Lerner et al. [6], ►- Abrahams and Marsh [7], ●-Malovichko et al. [8], ★-Iyi et al. [9]. Lattice parameter c: □-our results, △- [6], ▷- [7], ○ [8], ☆- [9]

Table

Lattice parameters a and c for the S1, S2, S3, S4 samples

Sample	C <sub>Li</sub> in the melt,	Latt. par. a, Å	Latt. par. c, Å
S1	48.2	$5,1501 \pm 2 \times 10^{-4}$	$13,8649 \pm 7 \times 10^{-4}$
S2	48.45	$5,1506 \pm 2 \times 10^{-4}$	$13,8673 \pm 7 \times 10^{-4}$
S3	50	$5,1497 \pm 2 \times 10^{-4}$	$13,8620 \pm 7 \times 10^{-4}$
S4	54.5	$5,1482 \pm 2 \times 10^{-4}$	$13,8599 \pm 8 \times 10^{-4}$

#### 4. Discussion and conclusions

The variation of the lattice constants has a similar behavior compared to the results obtained for undoped LN crystals [6-9]. This change demonstrates the dependence on the difference of the intrinsic defect concentration as it decreases with the increase of lithium content. Both lattice constants decrease with the increase of crystal stoichiometry, underlining the smaller concentration of intrinsic non-stoichiometric defects in the crystals with the compositions varying from

congruent to near stoichiometry. In addition, a slight decrease in the lattice parameters is noticed in Fe:LN crystals compared to the pure LN crystals with the same composition. One can assume that the main part of Fe ions occupies Li sites [13] which were captured by  $\text{Nb}^{5+}$  cations. In any case, this change is negligible compared to the change caused by the change in the intrinsic defects in the crystal due to the small amount of iron ions. Thus, the decrease of both lattice parameters  $a$  and  $c$  is caused by the decrease of intrinsic defects due to the change in the initial composition of the melt.

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**Ա.Վ. ԴԱՆԻԵԼՅԱՆ**

**ԵՐԿԱԹԻ ԻՈՆՆԵՐՈՎ ԼԵԳԻՐՎԱԾ ՏԱՐԲԵՐ ԲԱՂԱԴՐՈՒԹՅԱՄԲ  
ԼԻԹԻՈՒՄԻ ՆԻՈԲԱՏԻ ԲՅՈՒՐԵՂՆԵՐԻ ՑԱՆՑԻ ՊԱՐԱՄԵՏՐԵՐԻ  
ԲՆՈՒԹԱԳԻՐԸ**

Ռենտգենյան ճառագայթների դիֆրակցիայի կիրառմամբ ուսումնասիրվել են երկաթի իոններով լեգիրված տարբեր բաղադրությամբ լիթիումի նիոբատ բյուրեղի ցանցի պարամետրերը: Ստացված արդյունքները համեմատվել են անվանական մաքուր լիթիումի նիոբատի բյուրեղների դեպքում ստացված համանման պարամետրերի հետ:

**Առանցքային բառեր.** ռենտգենյան ճառագայթների դիֆրակցիա, լիթիումի նիոբատ, ցանցի պարամետրեր:

**А.В. ДАНИЕЛЯН**

**ХАРАКТЕРИСТИКА ПАРАМЕТРОВ РЕШЕТКИ КРИСТАЛЛОВ  
НИОБАТА ЛИТИЯ РАЗЛИЧНОЙ СТЕХИОМЕТРИИ,  
ЛЕГИРОВАННЫХ ИОНАМИ ЖЕЛЕЗА**

Исследованы параметры решетки кристаллов ниобата лития различной стехиометрии, легированных ионами железа, с использованием порошковой дифракции рентгеновских лучей. Результаты сравнены с аналогичными, полученными для номинально чистых кристаллов ниобата лития.

**Ключевые слова:** рентгеновская дифракция, ниобат лития, параметры решетки.