INFLUENCE OF THERMAL TREATMENT ON CRYSTAL AND MAGNETIC STRUCTURE OF NiO

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Abstract

The X-ray and neutron diffraction methods were used to investigate the influence of thermal treatment on crystal and magnetic structure parameters of NiO. The unit cell constant, the magnitude of unit cell and value of magnetic moment are dependent on thermal treatment.

1. INTRODUCTION

NiO crystallizes in the cubic NaCl-type crystal structure. The temperature dependence of susceptibility shows the antiferromagnetic properties below 520 K [1]. The neutron diffraction data indicates the magnetic ordering in which spins in (111) planes are parallel, while those in adjacent (111) planes are antiparallel [2]. In this paper the results of investigations of the crystal structure and magnetic properties of the NiO samples obtained at different temperatures are presented.

2. EXPERIMENT AND RESULTS

The samples of NiO were synthesised by the dehydratation of hydrooxide $Ni/OH/_2$ at following temperatures: 513, 563, 673, 873 and 1273 K. The obtained samples were checked by X-ray analysis using FeKα radiation and diffractometer DRON-3. NiO samples have cubic NaCl-type crystal structure.

Neutron diffraction patterns were obtained on a diffractometer at the RA reactor in Boris Kidrič Institute at Vinča using neutron wavelength of 0.128 nm in the room temperature.

In the neutron diffraction diagrams /see Fig. 1/ the strong reflections (hkl) of the nuclear origin and small peaks of magnetic origin $(\frac{hkl}{222})$ are observed. Refinement of the neutron diffraction data were carried out using the profile technique developed by Rietveld /3/. The refined parameters: the value of the lattice constant, half-height of the Bragg reflection (hkl), the value of the magnetic moment.

The half-height of the Bragg reflection H_{hkl} are given by the formula

$$H_{hkl} = H^{m}_{hkl} + H^{d}_{hkl} \tag{1}$$

where H^{m}_{hkl} are half-height of the Bragg reflection corresponding to magnitude of grain, H^{d}_{hkl} – the half-height of the Bragg reflection corresponding to deformation of unit cell. The first factor is given by the formula

$$H^{m}_{hkl} = \frac{K\lambda}{D_{hkl}\cos\theta_{hkl}} \tag{2}$$

where K is Scherrer constant, λ – wavelength of X-ray or neutron, D_{hkl} – the magnitude of grain, θ_{hkl} – the Bragg angle.

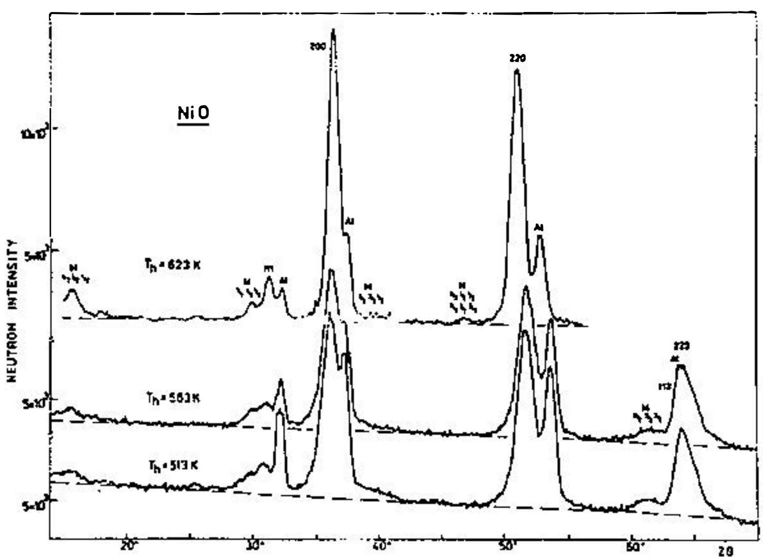

Fig. 1. A part of the neutron diffraction patterns of NiO measured at 300 K.

The second factor is given by the formula

$$H_{hkl} = 4 \left\langle \frac{\Delta a}{a} \right\rangle \operatorname{tg}\theta_{hkl} \tag{3}$$

where $\left\langle \frac{\Delta a}{a} \right\rangle$ is the deformation parameter of unit cell.

The relation /1/ with /2/ and /3/ givs the following equation:

$$\frac{H_{hkl}\cos\theta_{hkl}}{K\lambda} = \frac{1}{D_{hkl}} + \left\langle\frac{\Delta a}{a}\right\rangle \frac{4}{K\lambda}\sin\theta_{hkl} \qquad (4)$$

Using the formula /4/ the magnitude of grain and the deformation of the crystal and magnetic unit cell are determined /see Fig. 2/. The obtained values of these parameters are given in Table 1.

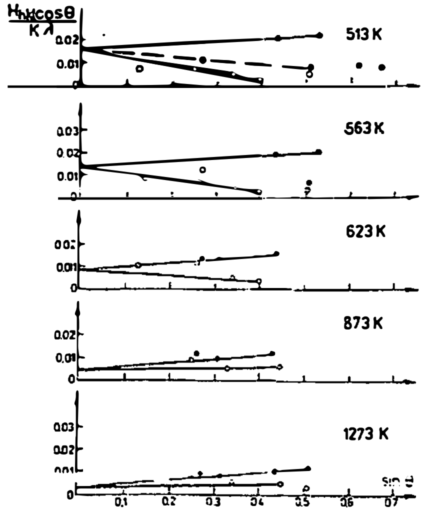

Fig. 2. Dependence of $\frac{H_{hkl}\cos\theta}{K\lambda}$ on $\sin\theta$ for NiO samples.

The increase in the temperature causes the following changes:

— decrease in lattice constant a,

— increase in magnitude of grain D_{hkl},

— the deformation of crystal unit cell $\left\langle\frac{\Delta a}{a}\right\rangle$ is constant,

— the deformation of magnetic unit cell decreases,

— increase in the value of magnetic moment.

Table 1. Structure and magnetic data of NiO

T_h/K/	a/nm/	μ/μ_B/	D_{hkl}/nm/	$\left\langle\frac{\Delta a}{a}\right\rangle$ cryst.	$\left\langle\frac{\Delta a}{a}\right\rangle$ magn.
513	0.4166/4/	1.68/54/	6.25	$4.3\ 10^{-2}$	$11.2\ 10^{-2}$
563	0.4177/7/	1.78/39/	7.14	$4.3\ 10^{-2}$	$5.3\ 10^{-2}$
623	0.4157/3/	1.79/27/	12.5	$4.6\ 10^{-2}$	$5.1\ 10^{-2}$
673	0.4142/8/	1.92/15/	18.0	$4.6\ 10^{-2}$	$4.8\ 10^{-2}$
873	0.4153/3/	1.83/23/	25.0	$5.3\ 10^{-2}$	$2.8\ 10^{-2}$
1273	0.4140/1/	1.89/16/	33.3	$4.6\ 10^{-2}$	$1.6\ 10^{-2}$

The obtained results indicate strong dependence of crystal and magnetic parameters on the temperature of the heating.

Ackonwledgements

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