The crystal structure of $NdGaO_3$ at 100 K and 293 K (F1/HASYLAB)

L.Vasylechko[1], L.Akselrud[2], W.Morgenroth[3], U.Bismayer[3], A.Matkovskii[1,4], D.Savytskii[1,4]

[1]SRC "Carat", 202 Stryjska St., Lviv 290031, Ukraine
[2] Lviv State University, 6 Kyryl and Mephodii St., Lviv 290005, Ukraine
[3] Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany Yourcity,
[4]State University "L'vivs'ka Politechnika", 12, Bandera St., 290646, Lviv, Ukraine

$NdGaO_3$ belongs to orthorhombically distorted perovskite-type compounds and is considered as a promising material for substrates for high-temperature superconducting thin layers. $NdGaO_3$ is stable in a wide temperature range and does not undergo phase transitions between 200 - 800 K. Near 200 K an anomaly in the thermal evolution of the dielectric loss, the magnetic susceptibility and the thermal expansion has been observed [1]. The determination of the crystal structure of $NdGaO_3$, both, at low and room-temperatures allows us to establish the nature of the anomalous thermal behaviour.

X-ray diffraction data were collected using the Kappa diffractometer at beam line F1 equipped with a SMART CCD system (axs) and an Oxford Cryostream cooling device. The measurement conditions were: λ = 0.496 Å, crystal-detector distance: 3.00 cm, omega scan mode ($\Delta\omega$ =0.1°, t=2s), saint parameters (xy/z integration box size): 2.0°/0.12°. A twin-free single domain plate-like shaped crystal was selected for the experiment. Typical FWHM value of reflections: 0.05°. An absorption correction was performed using SADABS [3].

Table 1. Crystallographic data for $NdGaO_3$ at 100 K and 293 K.

	100K	293K
Space group	P b n m	
a (Å)	5.3952(2)	5.4057(2)
b (Å)	5.4705(2)	5.4757(2)
c (Å)	7.6608(2)	7.6791(2)
Number of atoms in cell	20	
Absorption coefficient (1/cm)	160.31	
Radiation and wavelength	X-ray 0.49592	
Mode of refinement	F(hkl)	
Restrictions	F(hkl) > 4 σ (F)	
Weighing scheme	1/[σ(F)**2+0.0015F(obs)**2]	
Number of atom sites	4	
Number of free parameters	58	
Two-theta and sinΘ/λ (max)	74.48 1.220	74.64 1.223
Number of measured reflections	14508	17574
Number of independent reflections	1490	1424
R(%), R_W	3.91 3.47	4.44 4.02
Goodness of fit	1.010	1.160
Scale factor	0.814(6)	0.885(8)

The crystal structure determination [2] using the SMART software showed that $NdGaO_3$ crystallises at low and at room-temperature in the centosymmetric space group *Pbnm*. The data collection parameters are shown in Table 1. The analysis reveales that both structures differ considerably in the character of the thermal motions of the cations (Table 2). The Nd and Ga thermal ellipsoids at 100 K have opposite orientation compared with those at 293 K. The anharmonic thermal motions of Nd and Ga, calculated for

100 K and 293 K, are displayed by 4-rank polar tensors. The thermal anomaly of the physical properties of $NdGaO_3$ may therefore be well reflected by the thermal behaviour of the cations (Fig. 1).

Table 2. Positional and thermal parameters for $NdGaO_3$ at 100 K and 293 K.

	Nd		Ga		O1		O2	
	100 K	293 K	100 K	293 K	100 K	293 K	100 K	293 K
x/a	0.49087(2)	0.49092(4)	0	0	0.7098(2)	0.7107(3)	0.0803(4)	0.0800(5)
y/b	0.04268(2)	0.04142(4)	0	0	0.2092(2)	0.2097(3)	0.0181(3)	0.0174(5)
z/c	1/4	1/4	1/2	1/2	0.5426(2)	0.5422(2)	3/4	3/4
B(eq)	0.21(1)	0.42(2)	0.17(1)	0.31(2)	0.33(2)	0.47(2)	0.31(2)	0.46(3)
B11	0.25(2)	0.29(3)	0.15(1)	0.19(4)	0.35(3)	0.45(4)	0.39(4)	0.53(6)
B22	0.084(9)	0.67(3)	0.13(2)	0.53(4)	0.23(3)	0.48(4)	0.25(4)	0.63(6)
B33	0.29(2)	0.28(3)	0.24(3)	0.20(4)	0.40(3)	0.48(3)	0.27(4)	0.22(4)
B12	-0.024(4)	-0.050(7)	0.002(7)	0.00(1)	0.07(2)	0.16(3)	0.00(3)	0.00(4)
B13	0	0	0.01(1)	0.02(1)	0.03(2)	0.07(3)	0	0
B23	0	0	-0.02(3)	0.02(4)	0.01(2)	0.03(3)	0	0

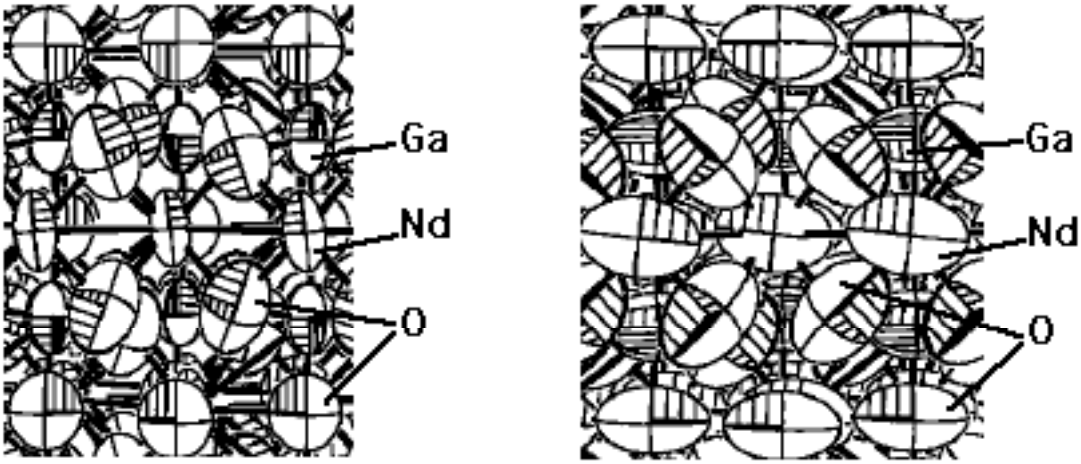

Fig. 1 Plot of $NdGaO_3$ structure normal to (100), 100 K (left), 293 K (right)

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