ADDITIONS AND CORRECTIONS

2005, Volume 109B

Yosuke Shiratori*, Arnaud Magrez, Jürgen Dornseiffer, Franz-Hubert Haegel, Christian Pithan, and Rainer Waser: Polymorphism in Micro-, Submicro-, and Nanocrystalline $NaNbO_3$

Page 20126. The *x* Na1 coordinate for NN@1000-12 indicated in Table 1 is corrected from 0.262(2) to 0.238(2). The corrected table is as follows:

TABLE 1

atom	*x*, *y*, *z*	biso (Å^2)	Wyck	site sym.	irreducible representations
		NN@1000-12, O_1, *Pbcm* (D_{2h}^{11}, no. 57)			
Nb	0.2429(4), 0.2627(4), 0.1252(5)	0.3(1)	8e	C_1	$3A_g + 3A_u + 3B_{1g} + 3B_{1u} + 3B_{2g} + 3B_{2u} + 3B_{3g} + 3B_{3u}$
Na1	0.238(2), 0.75, 0	0.7(1)	4c	C_2^x	$A_g + A_u + 2B_{1g} + 2B_{1u} + 2B_{2g} + 2B_{2u} + B_{3g} + B_{3u}$
Na2	0.258(3), 0.777(2), 0.25	0.7(1)	4d	C_s^{xy}	$2A_g + A_u + 2B_{1g} + B_{1u} + B_{2g} + 2B_{2u} + B_{3g} + 2B_{3u}$
O1	0.301(3), 0.25, 0	0.3(1)	4c	C_2^x	$A_g + A_u + 2B_{1g} + 2B_{1u} + 2B_{2g} + 2B_{2u} + B_{3g} + B_{3u}$
O2	0.174(4), 0.242(4), 0.25	0.3(1)	4d	C_s^{xy}	$2A_g + A_u + 2B_{1g} + B_{1u} + B_{2g} + 2B_{2u} + B_{3g} + 2B_{3u}$
O3	0.516(2), 0.019(4), 0.140(1)	0.3(1)	8e	C_1	$3A_g + 3A_u + 3B_{1g} + 3B_{1u} + 3B_{2g} + 3B_{2u} + 3B_{3g} + 3B_{3u}$
O4	0.967(2), 0.466(3), 0.113(1)	0.3(1)	8e	C_1	$3A_g + 3A_u + 3B_{1g} + 3B_{1u} + 3B_{2g} + 3B_{2u} + 3B_{3g} + 3B_{3u}$
	presence of an inversion center			Γ_{Total}	$15A_g + 13A_u + 17B_{1g} + 15B_{1u} + 15B_{2g} + 17B_{2u} + 13B_{3g} + 15B_{3u}$
				$\Gamma_{Acoustic}$	$B_{1u} + B_{2u} + B_{3u}$
lattice constants (Å)		reliability factors		$\Gamma_{Optical}$	$15A_g + 13A_u + 17B_{1g} + 14B_{1u} + 15B_{2g} + 16B_{2u} + 13B_{3g} + 14B_{3u}$
a	5.5071(1)	$R_p = 15.0$	$R_b = 5.7$	Γ_{IR}	$14B_{1u} + 16B_{2u} + 14B_{3u}$
b	5.5698(1)	$R_{wp} = 18.6$	$R_f = 9.5$	Γ_{Silent}	$13A_u$
c	15.5245(4)	$R_{exp} = 14.0$		Γ_{Raman}	$15A_g + 17B_{1g} + 15B_{2g} + 13B_{3g}$

10.1021/jp063704p
Published on Web 08/01/2006