

**substance: NiO**

**property: lattice parameter, thermal expansion**

**lattice parameter**

|     |          |                        |  |     |
|-----|----------|------------------------|--|-----|
| $a$ | 4.1705 Å | $T \rightarrow 0$ K    | variation with $T$ : Fig. 1, variation with pressure: Fig. 2                     | 71B |
|     | 4.1759 Å | $T = 298$ K            |  | 71B |
|     | 4.1758 Å | $T = 298$ K            |  | 54S |
|     | 4.1752 Å | $T = 273$ K            |  | 63P |
|     | 4.1767 Å | $T = 300$ K            |  |     |
|     | 4.1796 Å | $T = 354$ K            |  |     |
|     | 4.1886 Å | $T = 515$ K            |  |     |
|     | 4.1991 Å | $T = 688$ K            |  |     |
|     | 4.2070 Å | $T = 821$ K            |  |     |
|     | 4.2101 Å | $T = 890$ K            |  |     |
|     | 4.2183 Å | $T = 1023$ K           |  |     |
|     |          | $p_{O_2}$ [atm]        | samples quenched from 1673 K after equilibration at the pressures of $O_2$ shown | 69B |
|     | 4.1738 Å | $T = 298$ K, $10^{-6}$ |  |     |
|     | 4.1725 Å | $10^{-4}$              |  |     |
|     | 4.1719 Å | $10^{-2}$              |  |     |
|     | 4.1713 Å | $10^{-1}$              |  |     |
|     | 4.1701 Å | $10^{-0.7}$            |  |     |
|     | 4.1696 Å | $10^0$                 |  |     |

**coefficient of linear thermal expansion**

|          |                                     |                                    |     |
|----------|-------------------------------------|------------------------------------|-----|
| $\alpha$ | $3.2 \cdot 10^{-5} \text{ K}^{-1}$  | RT                                 | 66C |
|          | $7.93 \cdot 10^{-6} \text{ K}^{-1}$ | at high temperatures               | 71B |
|          | $1.39 \cdot 10^{-5} \text{ K}^{-1}$ | $T = 160 \dots 1300^\circ\text{C}$ | 63G |

**lattice parameter in Li doped NiO**

|     |          |                  |  |   |     |
|-----|----------|------------------|--|---|-----|
| $a$ |          | Li content [at%] |  | room temperature data for $p_{O_2} \leq 10^{-6}$ atm and incorporation of $Li_2O$ at 1073 K; at all concentrations $\alpha = 90.06^\circ$ | 76D |
|     | 4.1764 Å | 0                |  |   |     |
|     | 4.1758 Å | 1.00             |  |   |     |
|     | 4.1753 Å | 1.30             |  |   |     |
|     | 4.1746 Å | 1.70             |  |   |     |

At  $p_{O_2} = 10^{-6}$  atm the maximum Li content before segregation of a new phase is 1.9 at%. At higher  $p_{O_2}$  higher Li contents are possible [76D].

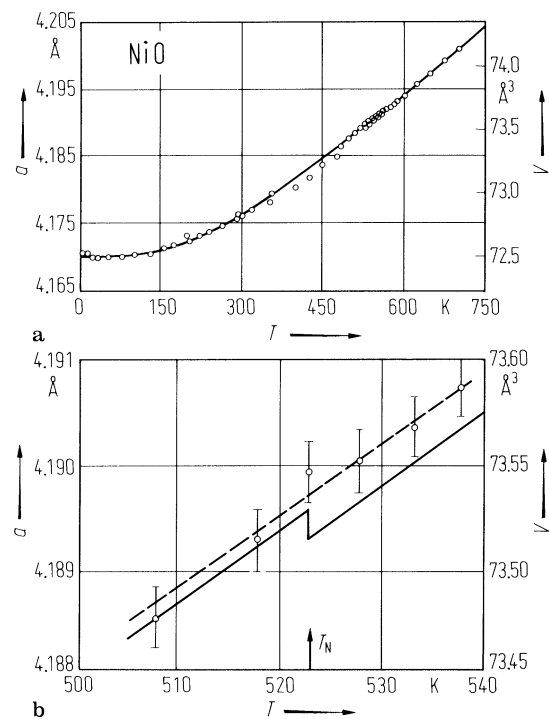
|     |         |       |          |   |     |
|-----|---------|-------|----------|---|-----|
| $a$ |         | x     | $\delta$ | third column gives x and $\delta$ in $Li_xNi_{1-x}O_{1+\delta}$ at RT | 66S |
|     | 4.170 Å | 0     | 0        |   |     |
|     | 4.167 Å | 0.005 | 0.057    |   |     |
|     | 4.164 Å | 0.025 | 0.063    |   |     |
|     | 4.153 Å | 0.075 | 0.078    |   |     |
|     | 4.140 Å | 0.135 | 0.097    |   |     |

## References:

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**Fig. 1.**

NiO. Lattice constant (volume of the unit cell) temperature. Solid curves calculated. Fig. b: solid curve: calculated lattice constants with magnetic contribution, dashed line: without that contribution [71B].



**Fig. 2.**

Variation of the lattice constant with pressure [66C].

