substance: NbO_2
property: crystal structure, thermal expansion, high-temperature modification

high-temperature form ($T \geq 800^oC$):

crystal structure: true rutile.

Differential thermal analysis reveals a marked endothermic anomaly at 795(5)°C [69S]. For rutile or pseudo-rutile unit cell parameters as a function of temperature: Fig. 1.

linear thermal expansion coefficients

α_a	$2.5 \cdot 10^{-6}$ K^{-1}	$T = 100^oC$	*a* and *c* are the pseudorutile	69S
α_c	$9.3 \cdot 10^{-6}$ K^{-1}		unit cell parameters for the	
α_a	$4.3 \cdot 10^{-6}$ K^{-1}	$T = 900^oC$	LT phase	
α_c	$24.5 \cdot 10^{-6}$ K^{-1}			

Diffuse superstructure lines may persist even up to 850°C [67S] suggesting that short-range structural fluctuations occur even well above the transition temperature [78P]. Furthermore, the superstructure lines of the low-temperature phase decrease continuously to zero, rather than discontinuously, suggesting a higher than first-order transition [74S]. Neutron diffraction studies on the lines lead to a crystallographic transition temperature of 808.5(1)°C [78P]. Very detailed studies of the transition [76P, 78P] have shown that the principal atomic displacements associated with the transformation may be represented as linear combinations of normal modes of the sort shown in Fig. 2 [76P, 78P]. However, all attempts to find a "soft mode" in the phonon spectrum have been unsuccessful and there remain some unresolved questions about the role of the lattice in the NbO_2 transition.

References:

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74S Shapiro, S. M., Axe, J. D., Shirane, C., Raccah, P. M.: Solid State Commun. 15 (1974) 377.
76P Pynn, R., Axe, J. D., Thomas, R.: Phys. Rev. B13 (1976) 2965.
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Fig. 1.

NbO_2. Rutile or pseudorutile unit cell parameters vs. temperature [69S].

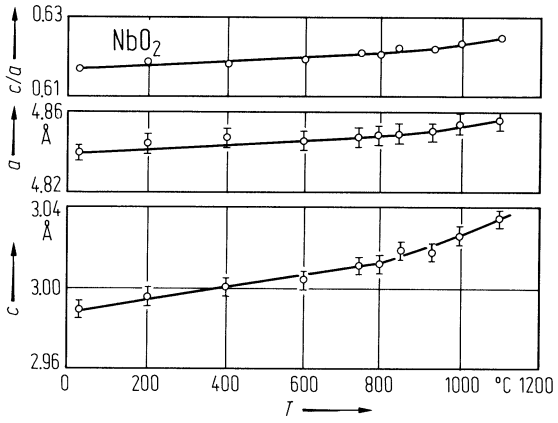

Fig. 2.

NbO_2. Normal modes of the lattice involved in the structural transition [76P, 78P].