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The structure of high-pressure tellurium

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Auszug

Ein kürzlich publizierter Vorschlag, daß die Hochdruck-Phase des Tellurs einer rhombisch-deformierten Struktur des β-Zinns entspricht, wird abgelehnt, weil beobachtete und berechnete Pulverdiagrammdaten zu stark voneinander abweichen.

Abstract

An orthorhombic distortion of the β-tin structure recently proposed for the high-pressure phase of tellurium must be rejected because it leads to gross discrepancies between the observed and calculated powder patterns.

VEZZOLI[1] recently proposed a structure for the high-pressure form of tellurium. This structure is the β-tin structure distorted by elongation of the b axis, so that it is orthorhombic rather than tetragonal. Lattice constants which were said to give the closest correspondence of calculated[1] to observed[2,3] spacings are $a = 5.831$ Å, $b = 7.650$ Å, $c = 2.680$ Å. No calculated intensities for this structure were included in the incomplete list of spacings tabulated by VEZZOLI. Spacings were accordingly recalculated out to $d > 1$ Å, and crude relative intensities were computed by multiplying the square of the geometric part of the structure factor by the multiplicity, and normalizing such that the smallest such product is unity. These "intensities" do not, of course,

[1] G. C. VEZZOLI, Proposed structure of high-pressure tellurium. Z. Kristallogr. **134** (1971) 305–307.

[2] S. S. KABALKINA, L. F. VERESHCHAGIN, and B. M. SHULENIN, [Phase transitions in tellurium at high pressures.] J. Exp. Theor. Physics **18**, 1422–1423; J. Eksperim. Teor. Fiziki (USSR) **45** (1963) 2073–2076.

[3] J. JAMIESON and D. B. MCWHAN, Crystal structure of tellurium at high pressure. J. Chem. Physics **43** (1965) 1149–1152.

Table 1. *Observed and calculated spacings and intensities*
(For definition of calculated "*I*", see text)

Calculated			Observed[3]		Calculated			Observed[3]	
hkl	*d*	"*I*"	*d*	*I*	*hkl*	*d*	"*I*"	*d*	*I*
020	3.825 Å	1						1.397	w
200	2.916	1	2.907 Å	vs	420	1.362 Å	2		
011	2.529	1			051	1.329	1	1.331 Å	vw
101	2.435	1	2.436	s	112	1.287	4		
220	2.319	2	2.364	m	060	1.275	1	1.277	vw
121	2.054	2			411	1.263	2		
040	1.912	1	1.923	w	341	1.215	2	1.228	w
211	1.911	2			251	1.209	2	1.190	vw
031	1.847	1	1.834	m	260	1.168	2		
			1.791	m	132	1.162	4	1.161	vw
240	1.599	2			440	1.159	2		
301	1.573	1			431	1.144	2		
231	1.560	2	1.555	vw	161	1.130	2	1.111	vw
141	1.504	2	1.491	vw	312	1.092	4		
400	1.458	1	1.456	m	501	1.069	1		
321	1.455	2			521	1.030	2		
					332	1.013	4	1.017	vvw

allow for Lorentz and polarization effects nor for normal decline, but can be used in the usual way for comparative purposes for spacings not differing too greatly. The results are summarized in Table 1. Agreement between observed and calculated spacings is not enough to suggest validity for a proposed structure. Equally important is the agreement between observed and calculated intensities. A point-by-point discussion of the discrepancies in Table 1 is unnecessary: These are so great that the proposed structure must be rejected.

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