Poster

High temperature single crystal X-ray diffraction of Pd bismuthides

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The phase transitions of PdBi and $PdBi_2$ structures were studied by *in-situ* high temperature single crystal X-ray diffraction.

Experimental diffraction data were collected starting from room temperature up to 573 K for PdBi, and 637 K for $PdBi_2$. The special experimental performing conditions were required due to high oxidation possibility of bismuth compounds. The crystals were capsulated in quartz glass capillaries which then were vacuumized.

The PdBi crystal was studied at the 373, 423, 473, 523 and 573 K temperatures. A phase transition near 500 K was observed. The structures of both polymorphic modifications were refined. The phase transition is characterized by symmetry transformation from space group $Cmc2_1$ to *Cmcm* (Table 1).

Table 1. Unit cell parameters for PdBi at high temperatures.

T (K)	Пр.гр.	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
373	$Cmc2_1$	8.7574(5)	7.2216(4)	10.6780(7)	675.30(7)
423		8.7775(6)	7.2297(5)	10.6847(7)	678.04(8)
473		8.8051(7)	7.2285(6)	10.6641(9)	678.80(10)
523	*Cmcm*	4.4208(3)	3.6162(9)	10.6446(4)	170.17(9)
573		4.4285(5)	3.6158(1)	10.6288(6)	170.19(7)

The $PdBi_2$ crystal was studied at the 373, 473, 573, 637 K temperatures. The monoclinic structure of alpha-$PdBi_2$ transformed into tetragonal beta-$PdBi_2$ near 600 K. Transformations of the structures at high temperatures were refined (Table 2).

Table 2. Unit cell parameters for PdBi at high temperatures.

T (K)	Пр.гр.	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	*V* (Å^3)
373	*C*2/*m*	12.7594(4)	4.2696(6)	5.6758(11)	102.41(1)	301.98(6)
473		12.792(2)	4.2766(4)	5.6819(6)	102.35(1)	303.65(6)
573		12.861(2)	4.2861(5)	5.6965(8)	102.51(2)	306.5598)
637	*I*4/*mmm*	3.3876(3)	3.3876(3)	13.092(2)		150.54(4)

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