X-Ray Study of the Compressibility of Hexagonal Selenium up to 15 kbar

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Abstract

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Corresponding Member of the Academy of Sciences of the USSR L. F. Vereshchagin, S. S. Kabalkina,
B. M. Shulenin

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The structure of tellurium and hexagonal selenium consists of infinite zigzag helical chains of atoms parallel to the axis c (structural type A8). The unit-cell parameters, atomic coordinates, shortest interatomic distances, and the valence angle between atomic bonds within the chain for each of these elements are presented in Table 1.

Studies of the thermal expansion of tellurium and hexagonal selenium (1) (Table 2) showed that both elements have a positive coefficient of linear expansion in the direction a and a small negative coefficient along c, as a result of which, upon heating, an increase in the parameter a and a decrease in c are observed, and consequently a decrease in c/a.

According to Bridgman' s data (2), under hydrostatic pressure up to 30 kbar a tellurium single crystal is stretched along the c axis and compressed along a ($\Delta c/c_0 > 0$; $\Delta a/a_0 < 0$). Later the same effect was observed radiographically up to 40 kbar (3). In the present work an analogous result was obtained under high hydrostatic pressure up to 15 kbar on hexagonal selenium.

Fig. 1. Dependence of the linear compressibility of selenium on pressure

Table 1

Element	a, Å	c, Å	x	Shortest interatomic distances, Å —in chain	Shortest interatomic distances, Å — between chains	Valence angle
Se (hex.)	4.36	4.95	0.217	2.32	3.46	105°
Te	4.45	5.91	0.269	2.86	3.74	102°

Fig. 2. Dependence of the ratio c/a for selenium on pressure. Fig. 3. Dependence of the volume compressibility of selenium on pressure. a —Bridgman' s data; b —our data.

Figure 1: Fig. 2. Dependence of the ratio c/a for selenium on pressure. Fig. 3. Dependence of the volume compressibility of selenium on pressure. a —Bridgman' s data; b —our data.

The X-ray investigation was carried out in a special chamber (4), in which the high-pressure vessel is a cone of metallic beryllium with a channel for the specimen (diameter 0.4 mm). Aviation gasoline was used as the pressure-transmitting medium; the pressure was recorded with a manganin manometer with an accuracy of ± 100 bar. The hexagonal modification of selenium was prepared from amorphous selenium at high pressure and temperature ($P = 60$ kbar, $t = 400°$). The results presented in Fig. 1 show that in the pressure interval $1 \div 15$ kbar in selenium there is

Table 2

Element	Coeff. of thermal expansion along the c axis, $\deg^{-1}$	Coeff. of thermal expansion along the a axis, $\deg^{-1}$
Se (hex.)	$-17.89 \cdot 10^{-6}$	$74.09 \cdot 10^{-6}$
Te	$-1.70 \cdot 10^{-6}$	$27.51 \cdot 10^{-6}$

there is a sharp anisotropy of compressibility, in character analogous to the anisotropy observed under the same conditions for Te: the crystal is strongly compressed in the direction of a and is slightly stretched along c; accordingly, c/a increases with pressure (Fig. 2).

This unusual anisotropy of the compressibility of selenium and tellurium can be explained if one recalls that a structure of this type is easily obtained by compressing the closest cubic packing of spheres along a threefold axis (5): as a result, the parameter c is considerably reduced while a simultaneously increases; c/a decreases by about a factor of 2—from 2.45 for the cube to 1.14 in the case of hexagonal Se and to 1.33 in the case of Te. From this point of view, high pressure as it were gradually removes the "initial distortion" of the structures of the elements considered, as a result of which their structure approaches the cubic one.

Fig. 2. Dependence of the ratio c/a for selenium on pressure
Fig. 3. Dependence of the volume compressibility of selenium on pressure. a —Bridgman' s data; b —our data

The linear compressibilities (Table 3) and the coefficients of thermal expansion (Table 2) of Se are larger in absolute magnitude. It is therefore natural to suppose that the bond between neighboring atoms in one chain in selenium must be weaker than in tellurium.

Table 3

Element	P, kbar	$-\Delta c/c$, %	$-\Delta a/a$, %
Se (hex)	15	-0.5	6.0
Te	15	-0.4	2.9

The values of $\Delta V/V_0$ at various P obtained in this work agree fairly well with Bridgman' s data (6) (Fig. 3).

Institute of High Pressure Physics
Academy of Sciences of the USSR

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Note: Figure translations are in progress. See original paper for figures.