OBTAINING DENSE MODIFICATIONS OF GERMANIUM AND SILICON UNDER CONDITIONS OF THE SIMULTANEOUS ACTION OF HIGH PRESSURE AND SHEAR STRESS

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Abstract

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OBTAINING DENSE MODIFICATIONS OF GERMANIUM AND SILICON UNDER CONDITIONS OF THE SIMULTANEOUS ACTION OF HIGH PRESSURE AND SHEAR STRESS

At the present time, much attention is being given to studies of the behavior of germanium and silicon under pressure. New dense modifications have been found, and their phase diagrams are being studied. Thus, Wentorf and Kasper ([1]) found a new dense modification of silicon under conditions of the simultaneous action of high pressures and shear stress and determined the crystal structure of Si_{III} as a body-centered cube with parameter $a = 6.64$ Å. Bundy and Kasper ([2]) investigated germanium at room temperature and obtained the dense modification of germanium Ge_{III} by compressing ordinary cubic germanium to 120 kbar. They determined the crystal structure of germanium as tetragonal, with parameters $a = 5.93$ Å and $c = 6.98$ Å. Investigation of the phase diagrams of germanium and silicon ([3,4]) confirmed the existence of the Ge_{III} and Si_{III} phases, but so far it has not been possible to outline the regions of existence of these dense modifications.

The authors of the present article carried out studies of the behavior of germanium and silicon under pressure with the simultaneous application of shear stress. The essence of this method is that, if a specimen under pressure and shear stress undergoes any chemical or phase transformations, these transformations are accompanied by an abrupt change in the magnitude of the shear stress. This method of investigation is attractive because of its relative simplicity and, at the same time, high sensitivity, since it makes it possible to record phase transitions that cannot be detected by the piston-displacement method because of an excessively small change in volume.

The investigations were carried out on an apparatus constructed at the Institute of High Pressure Physics of the Academy of Sciences of the USSR ([5]). The apparatus was calibrated by the polymorphic transitions in bismuth, thallium, and barium. Germanium specimens were subjected to compression up to 120 kbar, and silicon specimens to 200 kbar, with simultaneous application of shear stress at room temperature. After the pressure was released, X-ray structural

analysis of the specimens was carried out; it showed that, in germanium and silicon, an irreversible phase transition into the dense modifications Ge_{III} and Si_{III} had occurred.

The tetragonal modification of germanium Ge_{III} was obtained under conditions of applied shear stress during compression to 100 kbar and at room temperature, with holding under these conditions for no more than 3 hours, and was detected radiographically after the pressure had been reduced to atmospheric.

On X-ray diffraction patterns of germanium taken with copper radiation using a nickel filter, 29 lines of the new modification of germanium were found. This modification was determined to be tetragonal, with parameters $a = 5.93 \pm 0.02$ Å and $c = 6.98 \pm 0.02$ Å.

From the extinction rules, the space group was determined as $P4_32_12$ (D_4^8). The X-ray density was calculated to be 5.91 for 12 atoms per unit cell. The indexing was carried out using Hull charts and analytically.

The dense modification of silicon was obtained under conditions of applied shear stress during compression to 170 kbar and at room temperature.

with a holding time also of no more than 3 hours, and was detected by X-ray structural analysis after the pressure had been reduced to atmospheric.

On X-ray photographs of silicon, also taken in copper radiation with a nickel filter, 22 lines of the new modification of silicon were found. This modification was identified as a body-centered cube with parameter $a = 6.64 \pm 0.02$ Å. The indexing was carried out analytically.

It was noted that the transition to the dense modifications Ge_{III} and Si_{III} depends to a considerable extent on the method of applying pressure and shear stress. The best results at comparatively short holding times were obtained by gradually loading the samples with the gradual application of shear stress. Complete transition to the dense modifications was obtained by increasing the number of stages to 25 and by subsequent holding under pressure and shear stress for 3 hours.

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