FISH P65 0734

Reprinted from

PHYSICS LETTERS

Volume 16, number 1, 1 May 1965

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pp. 26 - 27



NORTH-HOLLAND PUBLISHING COMPANY AMSTERDAM Volume 16, number 1

PHYSICS LETTERS

THE EXCITATION SPECTRUM OF BORON IN SILICON UNDER UNIAXIAL STRESS *

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Received 3 April 1965

Several investigators have studied the excitation spectrum of neutral boron in silicon [1-3]. In order to determine the symmetries of the energy levels involved in the optical excitations, we have observed the spectrum of boron in silicon subjected to a uniaxial compression. Such a determination is of particular interest for acceptors in silicon since the energy correlation between the experimentally determined excited states and those calculated by Kohn and Schechter [4, 5] is not satisfactory.

The experimental results for the compressive force, F, parallel to [111] and for F = 0 are presented in fig. 1. Similar results have been obtained for F[110] and F[100]. The uniaxial compression was applied by the use of the differential thermal contraction technique described by Rose-Innes [6]. The spectra were examined with polarized radiation, the electric vector, E, being either parallel or perpendicular to F. Fig. 1a shows part of the spectrum for F = 0. The excitation lines are labelled using the notation of Colbow [3]. The high energy shoulder of line 4 observed by Colbow is resolved in the present measurements as can be seen in the inset to fig. 1a. This is designated by 4A, and occurs at an energy of 39.90 ± 0.04 MeV. Only the lines 1, 2, 3 and 4 have been examined under stress as the resulting components for these could be identified with least ambiguity.

As can be seen from fig. 1b, $F \| [111]$, each of the strong lines 2 and 4 gives rise to a total of four stress-induced components. The intensity of the components is strongly dependent upon the direction of polarization, the components 2.1 and 2.4 and 4.2 and 4.4 being observed only for $E \| F$ whereas 2.2 and 2.3 and 4.1 and 4.3 appear only for $E \perp F$. The results given for line 1, show only those components which appear for $E \perp F$. In this direction of polarization, three components were observed. For $E \| F$ several very weak components were observed; however, for this direction of polarization, with the grating used, the intensity was marginal. In view of the small intensity of line 3, it is difficult to establish the total number of stress-induced components, the only line clearly observed being the high energy component in $E \perp F$.

The effective mass calculations [4,5] show that the hole states are either two- or four-fold degenerate. The effect of a uniaxial stress is to split the four-fold states into two two-fold states without affecting the degeneracy of the two-fold states [4]. The ground states is believed to be four-fold degenerate. Hence transitions to two-



Fig. 1. (a) The excitation spectrum of boron doped silicon for zero stress with liquid helium as coolant. (b) The excitation spectrum of boron-doped silicon for compression, F, along [111]. The room temperature resistivities of both samples lie in the range 10-15 Ω cm.

^{*} Work supported in part by the Office of Naval Research, and the U.S. Army Research Office, Durham.

Volume 16, number 1

fold states should exhibit a maximum of two com-

ponents only, while those to four-fold states may give rise to four components.

The present experimental results interpreted in the above framework, clearly establish that the prominent lines 2 and 4 have four-fold degenerate final states. For $F \parallel [111]$, line 1 exhibits three components; on this basis line 1 must also have a four-fold degenerate final state. For line 3, no more than two components have been observed in any of the three directions of compression examined. In view of this, it is tentatively suggested that this line has a two-fold degenerate final state. The present results and their interpretation have clearly demonstrated the importance of making observations with more than one direction of compression.

The above interpretation is based on the assumption that the ground state is four-fold degenerate. The populations of the stress-induced ground states will be a function of the magnitude of the stress as well as the sample temperature. Such effects have been observed. An investigation of the temperature dependence of the intensities of the stress-induced components at a given stress is an unambigous means of identifying which ground state is involved in a given transition.

The energy spacing of 4.1 MeV between lines 1 and 2 (the lines of lowest energies) is in reasonable agreement with the calculated spacing [5] of 3.9 MeV ($B^* < 0$) for the two lowest excited states. Further, the theory predicts a four-fold degeneracy for these states, in agreement with the present results. The remaining two states calculated by Schechter [5] are both two-fold degenerate. Thus neither of these states can be the final state of line 4. Hence there is clear need to extend the effective mass calculations for acceptors in silicon to include at least the 3p-like states as has been done by Mendelson and James [7] for germanium.

The polarization features observed for the different directions of compression may be understood from symmetry considerations. Details of this with more extensive experimental investigations for different directions of stress and direction of light propagation will be presented elsewhere.

The authors wish to thank Professor H. J. Yearian for orienting the crystals and Miss Louise Roth and C. D. Wilson for assistance in preparation of the samples.

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PHYSICS LETTERS

1 May 1965



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LARGE-GRAINED ALPHA PLUTONIUM PRODUCED UNDER EXTREME PRESSURE (Roland B. Fischer, Rocky Flats)

Theoretical considerations lead to a conclusion that at sufficiently high pressures, plutonium might exist only as alpha phase below the melting point. This provides the interesting possibility of allowing plutonium to solidify slowly under pressure directly into alpha phase. Thus, large grains of alpha plutonium might be produced for study.

Recent work at Rocky Flats supports the above hypothesis. Compared to the ordinary alpha microstructures, the new type of microstructure is far better defined and consists of large grains. Columnar grains about 10 mils in diameter and 60 mils in length have been produced. An example of one specimen is shown in Figure 1. Undoubtedly, larger grains or crystals can be produced in larger high pressure cells.

The specimens of large-grained alpha were produced by heating plutonium to about 560°C under a pressure of about 60 to 70 kilobars. The metal was cooled slowly while under pressure. An effort was made to maintain a sharp thermal gradient along the specimen.

By means of hot-stage microscopy, movies have been taken of the alpha-to-beta-to-alpha transformations as revealed by the topography of polished large-grained specimens. The alpha-to-beta transformation moved intermittently as an irregular-fronted wave across the grains, stopping or changing direction at grain boundaries. On return to the alpha phase, the specimen retained ghost images of the original alpha grains. This is an example of such studies as can be made on the new type of microstructure.

Back-reflection Laue patterns of the grains show that the specimens are in a strained condition after removal from the high-pressure cell. A five-hour heat treatment at 115°C appeared to relieve the strain because sharper Laue patterns were obtained after such treatment.

Future work includes an effort to make even larger alpha grains and to conduct basic studies on them.



FIGURE 1

Polarized—light photomicrograph of a large—grained alpha plutonium specimen prepared under high pressure.