rf magnetic field vectors was parallel to most of the graphitic planes in the powder particles.

The derivative of the absorption with respect to dc magnetic field strength was recorded point by point with a microwave spectrometer similar to Yale University's instrument. The crossover values for the observed resonances are reasonably constant, having the mean g value of 2.0056 ± 0.002, based on 2.0036 for powdered picryl hydrazyl. The accuracy of cross-over location is limited by the asymmetry which is quite uniform for all the samples reported here.

The widths, defined for convenience as the separation between points of maximum signal, are given in units of the static magnetic field. The static magnetic field is measured by the proton resonance in USP mineral oil. The modulation amplitude was in each case less than one-third the observed width.

Figure 1 shows what heat treatment of a soft carbon powder does to the width of the spin resonance absorption. The two regions of increased width occur near 1700°C and 2400°C.

According to recent measurements,[3] the Hall coefficient R of a soft carbon solid goes through zero near 1750°C and near 2350°C. The two pairs of Ht values suggest that there is a mechanism of broadening for the spin resonance which produces an increased line width when the densities of electrons and holes are approximately equal. The two cases of heat treatment (near 1700 and 2400) are otherwise quite different with respect to the filling and structure of the electronic energy bands.[4]

Quite recently, resonance absorption in solid carbon samples has been observed with g values of 2.005 ± 0.002. The relation of heat treatment to structure for powders and for solid carbons is being studied.

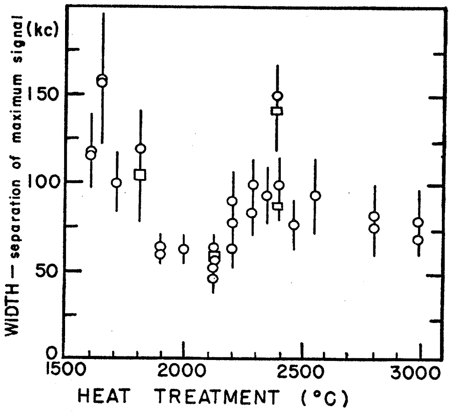

FIG. 1. Paramagnetic resonance absorption in soft carbon powder at 3 cm as a function of the temperature of heat treatment. Circles indicate powder suspended in polystyrene; squares, same powder loose in plastic bag; vertical bars, extreme allowances for error due to bluntness of observed shapes of the first derivative signal.

The author is grateful to Dr. S. Mrozowski for his stimulating interest and helpful advice, to Mr. D. Wobschall for his aid in constructing and operating the spectrometer, to Dr. R. Beringer for the loan of several crucial components of the spectrometer, and to Dr. M. A. Garstens for the gift of the hydrazyl.

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Speculations on the Energy Band Structure of Ge – Si Alloys

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JOHNSON and Christian[1] of these Laboratories have recently reported on some of the properties of Ge-Si alloys. The optical energy gap *vs* composition (see reference 1, Fig. 3) exhibits the following characteristics: In the range 0 to 15 mole percent Si, the gap increases linearly from 0.72 to 0.94 ev. A break then occurs, and the gap continues to increase, reaching 1.2 ev at pure Si. We may ask: What is the energy band structure of a Ge-Si alloy of given composition, and what is the explanation of the break in the curve described above?

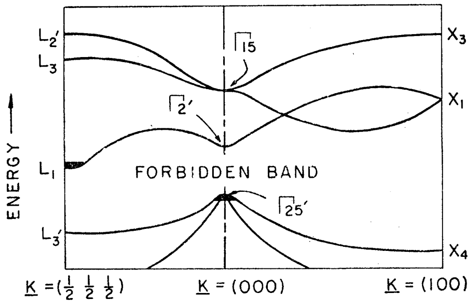
Alloys have energy bands with a high density of states and bands with a low density of states.[2] In a Ge-Si alloy, the former should resemble the allowed bands of a perfect germanium or silicon crystal according as the predominant constituent of the alloy is germanium or silicon.

Schematic diagrams of the band structures of perfect germanium and silicon crystals are shown in Figs. 1a and 1b, respectively. Figure 1a was suggested by the preliminary results of a new theoretical investigation of the band structure of the germanium crystal[3] and by the results of cyclotron resonance experiments.[4] The conduction band structure of Fig. 1b was obtained by distorting the conduction bands of Fig. 1a so as to bring the [100] minima below the [111] minima. The conduction band structure of Fig. 1b is consistent with the results of piezoresistance measurements on n-Si by Smith[5] and with unpublished magnetoresistance data on n-Si by Pearson.[6] The valence band structure of Fig. 1b was suggested by recent cyclotron resonance absorption measurements on silicon by Lax and Dexter.[7]

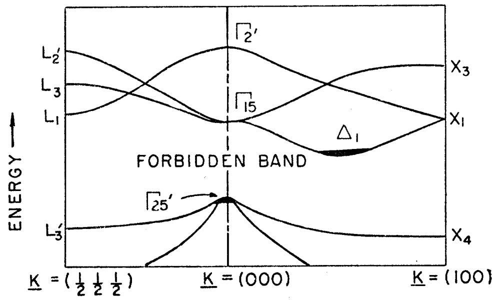
We now make the following assumptions: (1) The addition of silicon to germanium affects the form and relative disposition of all valence and conduction bands. However, the changes produced in the conduction band structure are more radical than those involving the valence band structure. (2) As the silicon content increases, the conduction band having [111] minima is raised relative to the conduction band having [100] minima. Both of these conduction bands move away from the valence bands, the lowest conduction band at a faster rate than the next-to-the-lowest conduction band. (3) The top of the valence band structure remains at the central point of the reduced zone over the entire range of alloy composition. (4) The optical absorption edge is determined by nonvertical electronic transitions over the entire range.

Referring now to reference 1, Fig. 3 [E_{gap} *vs* mole percent Si], we suggest that electrons occupy states at the [111] minima in the range 0 to about 15 mole percent Si. In the region of the break in the E_{gap} *vs* mole percent Si curve, the [100] and the [111] minima are both populated. These minima are here separated in energy by a quantity of the order of kT. As the silicon content is increased above about 15 mole percent, the [111] minima are pushed above the [100] minima.

The optical absorption edge, i.e., the measured energy gap, is thus determined by electronic transitions from valence band states near $k=(000)$ to the conduction band states near $k=(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ in the range 0 to 15 mole percent Si. The absorption edge in the range above 15 mole percent Si is determined by transitions from the top of the valence band to states at the bottom of the conduction band, which here lie along the [100] axes.



(a) PURE GERMANIUM



(b) PURE SILICON

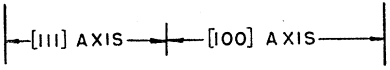


FIG. 1. a and b. Schematic diagrams of energy band contours in perfect germanium and silicon crystals along [111] and [100] axes in the reduced zone. States normally occupied by electrons and holes at room temperature are shown darkened. The symbols give the symmetry classification of the various states in the notation of reference 3. The removal of degeneracy by spin-orbit interaction is not shown.

It is conceivable that these ideas could be verified by performing magnetoresistance or cyclotron resonance measurements on single-crystal suitably-doped Ge-Si alloys of varying compositions. (Johnson and Christian[1] report that single crystals have already been produced in the range 0 to 12.6 mole percent Si.) Magnetoresistance measurements on both *n*- and *p*-type single Ge-Si alloy samples have been initiated at these Laboratories. It is hoped that these experiments will bear out the speculations presented above.

It has occurred independently to Paul and Brooks[8] and to the author that the application of high pressure to perfect single crystals of germanium could raise the [111] minima above the other minima, i.e., above the [100] minima or the (000) minimum. Dr. R. H. Parmenter of these Laboratories is currently engaged in a theoretical study of the modifications in the band structure of germanium produced by changes in lattice constant or addition of silicon atoms.

The author wishes to thank Dr. D. O. North and Dr. R. H. Parmenter of the RCA Laboratories for stimulating conversations. The author is grateful to Dr. B. Lax, Dr. R. N. Dexter, and Dr. H. J. Zeiger of the Lincoln Laboratory, Massachusetts Institute of Technology; Dr. C. Herring and Dr. G. L. Pearson of the Bell Telephone Laboratories; and Professor H. Brooks and Dr. W. Paul of Harvard University for discussing their work with him prior to publication.

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[4] Dresselhaus, Kip, and Kittel, Phys. Rev. **92**, 827 (1953); Lax, Zeiger, Dexter, and Rosenblum, Phys. Rev. **93**, 1418 (1954); R. N. Dexter *et al.*, Phys. Rev. (to be published).

[5] C. S. Smith, Phys. Rev. **94**, 42 (1954).

[6] G. L. Pearson (private communication); see also G. L. Pearson and C. Herring (to be published). Dr. Herring discussed the significance of Pearson's data and of Smith's results at the Stanford Meeting of the American Physical Society, December, 1953, Invited Paper C1.

[7] Dr. B. Lax has just informed the writer that the top of the valence band in silicon appears to lie at the central point of the reduced zone, and to have a form similar to that in germanium. Lax and Dexter's data on silicon also indicate that the states normally occupied by electrons lie along the [100] axes in the reduced zone.

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Electrical Conductivity of Magnesium Oxide Single Crystals

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MEASUREMENTS of the electrical conductivity of magnesium oxide have been performed by two or three investigators. Lempicki[1] made measure-