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# INFRARED SPECTRA OF HEAT TREATMENT CENTERS IN SILICON

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Oxygen dissolved in silicon at temperatures near the melting point forms a neutral unit with two silicon-oxygen bonds.[1,2] On heating near 1000°C the oxygen precipitates into an $SiO_2$ phase.[3] Heat treatment in the temperature range 300-600°C produces donors[4] which apparently result from some step preliminary to the precipitation process. The electrical properties are complicated,[4] and Hall effect measurements[5] have indicated several donor levels. Other results[3] indicate that the heat treatment donor is an $SiO_4$ complex. We have observed electronic transitions of heat treatment centers optically. These results give direct information about such centers and provide some insight into the atomic rearrangements occurring during heat treatment.

The samples used were saturated with oxygen at 1420°C ($1.8\times10^{18}$ atoms/cm$^3$) and contained no detectable concentration of other donors. Infrared spectra at 4.2°K were obtained for heat treatment donor concentrations, $n$, varying from $2.5\times10^{14}$/cm$^3$ to $6.5\times10^{16}$/cm$^3$. $n$ was determined from the measured room-temperature conductivity using the mobility data of Prince.[6] Figure 1 (a) shows the spectra at 300°K and 4.2°K for $n=10^{15}$/cm$^3$. The band near 515 cm$^{-1}$ is the Si-O bending vibration.[2] The absorptions which appear on cooling have a temperature dependence similar to that observed for other shallow donor impurities. These are electronic transitions from the ground state to excited states of a heat treatment center. Heating this sample to 630°C reduced $n$ to $2.5\times10^{14}$/cm$^3$, and the spectrum shown in Fig. 1 (b) was obtained. The intensities of the electronic transitions have decreased by a factor of four as has $n$. For $n\leq10^{15}$/cm$^3$ no absorptions were observed at lower energies.

Fig. 1 (c) shows the spectrum of arsenic, which has a term scheme in agreement[7] with that calculated for donors by Kohn and Luttinger.[8] The strong bands at 0.0423 and 0.0475 ev are, respectively, the $1s\rightarrow2p$, $m=0$ and $1s\rightarrow2p$, $m=\pm1$ transitions. Fig. 1 (a) also shows two strong bands with approximately the same separation. The energies of these transitions and the theoretical separations[8] of the $2p$ levels from the conduction band give an approximate ionization energy, $E_0$, of 0.066 ev. The spectral pattern in Fig. 1 (a) is quite different from that of As indicating that the potential energy for this heat treatment center does not have the spherical symmetry of the Coulombic potential used in the effective-mass approximation.[8]

The intensities of the 0.066-ev donor absorptions are directly proportional to $n$ below $10^{15}$/cm$^3$. However, these intensities give $0.4n$ for the 0.066-ev donor density, $n_1$, at $n=10^{16}$/cm$^3$ and indicate that $n_1$ approaches $10^{16}$/cm$^3$ for higher values of $n$. As $n$ is increased by heating at 430°C, new bands also appear at lower energies. Figure 2 illustrates the results for $n=4\times10^{16}$/cm$^3$. Thirty absorptions were resolved altogether between 510 and 300 cm$^{-1}$ in the spectra for samples with various amounts of heating at 430°C. No one spectrum shows all of these bands. Bands observed after heating at 430°C are removed by heating at 630°C and obtained again after further heating at 430°C.

Newman[9] has shown that the intensities of shallow acceptor bands are essentially linearly dependent on acceptor density, $p$, up to about $5\times10^{16}$/cm$^3$ and that the major effect of increas-

ing $p$ is a broadening of the bands which begins at $p \approx 10^{16}/\text{cm}^3$. Assuming similar behavior for shallow donors, our results indicate that oxygen produces several discrete heat treatment centers which can be formed by the clustering of small numbers of oxygen atoms during heating near 450°C. The observed bands can be separated into four distinct groups, each with its own energy level scheme. These are not identical but are more similar to each other than to the Kohn-Luttinger scheme. Each pattern has two strong lines with separations close to the calculated $(2p, m=\pm 1)$-$(2p, m=0)$ spacing[8] which permit estimates of $E_0$ of 0.066, 0.056, 0.052, and 0.045 ev.

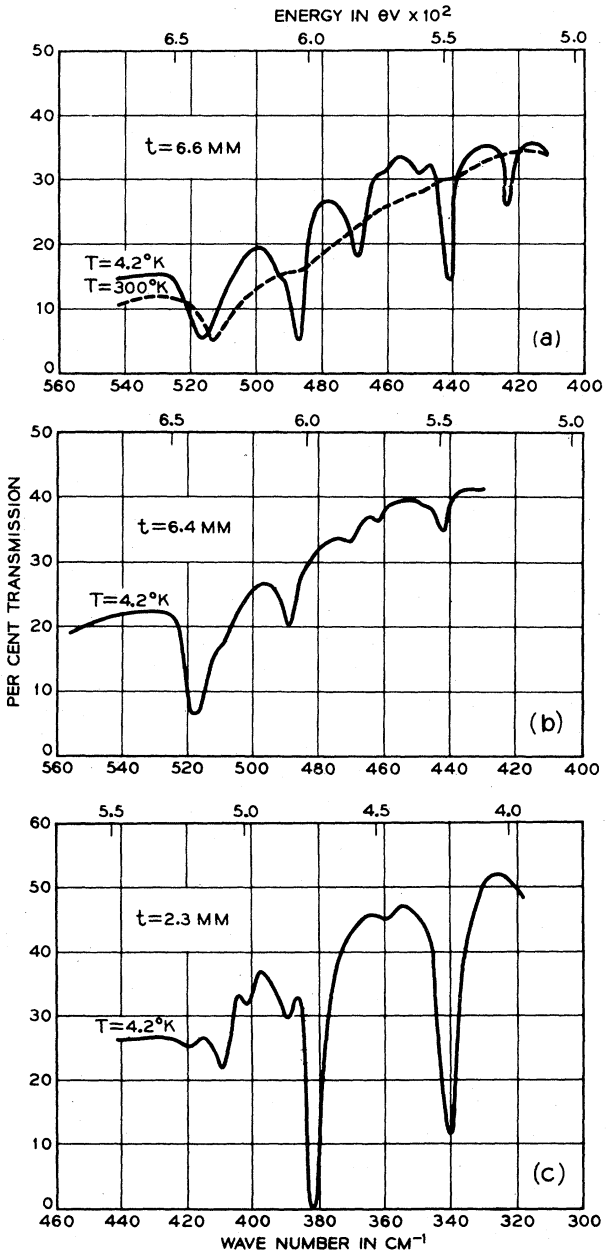


FIG. 1 Electronic spectra of (a) heat treatment centers, $n = 10^{15}/\text{cm}^3$, (b) heat treatment centers, $n = 2.5 \times 10^{14}/\text{cm}^3$, and (c) arsenic in silicon, $n = 2 \times 10^{15}/\text{cm}^3$.

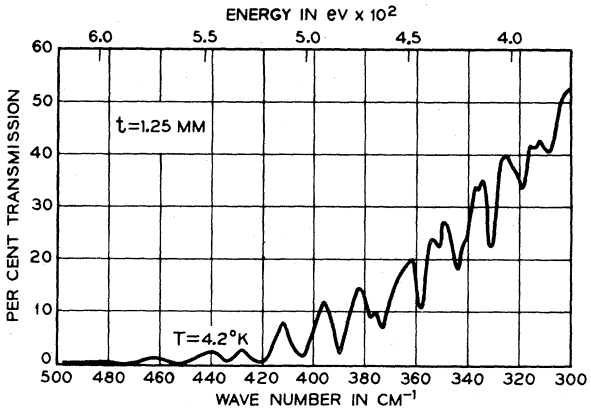


FIG. 2. Electronic spectrum of heat treatment centers in silicon for $n = 4 \times 10^{16}/\text{cm}^3$.

Although the nature of these centers has not been definitely established, further investigation of the energy level schemes and the kinetics of heat treatment are in progress

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## EFFECTS OF ATOMIC ELECTRONS ON $p$-$p$ AND $n$-$p$ SCATTERING*

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Early estimates of the effect of screening have shown it to be small.[1] Recent improvements in