the light-scattering spectra of the crystalline solids $KTaO_3$ and $SrTiO_3$ exhibit two temperature-dependent dynamic central pekas. Neither behaves in a singular manner upon approach to the known structural phase transitions in these materials. The narrower peak is rather firmly established as due to scattering from entropy fluctuations, with an expected but previously unobserved enhancement due to the direct temperature dependence of the polarizability at constant density. The broader peak exhibits a strongly temperature-dependent linewidth and is tentatively identified as arising from two-phonon processes. What connection, if any, these dynamic central peaks have with the frequently reported unresolved central peaks in phase-transition studies is now being explored in other crystals.

We are grateful to P. C. Hohenberg for helpful discussions and to H. L. Carter for assistance in various phases of the experiment.

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Formation of the Upper Hubbard Band from Negative-Donor-Ion States in Silicon

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The spectral response from shallow negative donor ions in silicon has been studied over a range of donor concentrations between 1×10^{14} and 1×10^{17} cm^{-3}. At low donor concentrations the binding energy of the negative-ion state is well described by the effective-mass theory. The formation of the upper Hubbard band out of these states is observed at a donor concentration of 3×10^{15} cm^{-3}—about three orders of magnitude lower than the concentration at which the metal-insulator transition occurs in this material.

In this Letter I would like to report the first experimental observation of the onset of formation of the upper Hubbard band in an impurity-doped semiconductor. The upper and lower Hubbard bands are formed out of impurity-state wave functions when the concentration of impurities in the material is sufficient to produce a critical overlap of the wave functions from adjacent impurity atoms. The familiar metal-insulator transition in these materials occurs at still higher concentrations when the upper and lower Hubbard bands overlap each other,[1] giving a continuous spectrum of unoccupied states in which the impurity electrons can move. Transitions between the upper and lower Hubbard bands have been observed previously, for example in the hopping-conductivity activation energy ϵ_2,[2] and in optical absorption and photoconductivity[3] resulting from excitation of electrons from the lower band into the upper band. In this Letter I will present data on the excitation of electrons from states in the upper band into the conduction band. The onset of the formation of the upper Hubbard band is observed from the spectral properties of the photoconductive signal when submillimeter radiation is used to photoexcite electrons which have been optically pumped into the upper Hubbard band. The existence of a band is shown by the change in the shape of the spectral response as the temperature is varied over a range such that the photoexcitation process is forced to compete with thermal excitation. Finally, the lowest states within the band are determined from the temperature dependence of the photoconductive signal using a submillimeter laser source at 118 μm.

The experiments reported here were carried out in uncompensated silicon doped with phosphorus or arsenic impurities having impurity concentrations between 10^{14} and 10^{17} cm^{-3}. These impurities have electron binding energies of 46 and 54 meV, respectively, in lightly doped samples, and the general features of the impurity states are given by the effective-mass theory which describes them as hydrogen atoms with an electron effective mass $m^* = 0.30 m_0$ immersed in the dielectric medium of the silicon crystal, $\epsilon = 11.47$. The lower Hubbard band is formed by the overlap of the ground states of the impurity wave functions, and in silicon this has been observed to occur experimentally from hopping conduction which is detected for samples doped on the order of 1×10^{17} cm^{-3}.[4] The upper Hubbard band is associated with electron states which have two electrons on a site, while the lower Hubbard band involves only one electron per site. Thus, the upper Hubbard band is formed from the overlap of the negative-ion states of the impurities, referred to as D^- states. Within the upper Hubbard band the random potential fluctuations due to the random distribution of donors and acceptors will localize states in the lower part of this band. Electrons bound to local potentials will have energies between the bottom of the band and the so called "mobility edge" as described by Anderson.[5] In the same manner as the effective-mass theory describes the neutral-donor states, the negative-donor-ion state is predicted to have a binding energy of 1.7 meV in silicon, based upon the 0.747-eV binding energy of the atomic H$^-$ state. Since the negative donor ion is spatially larger than the neutral donor, overlap of the negative-donor-ion wave functions is expected to occur at a lower concentration than that required for overlap of the wave functions of neutral impurities.

To probe the upper Hubbard band, electrons were first excited from neutral donor impurities into the conduction band with 300-K radiation. The concentration of electrons in the conduction band in steady-state conditions is typically 10^8–10^{10} cm^{-3}. At temperatures below 4 K some of these electrons are captured by neutral donors which thus become negative donor ions. At low concentrations the negative-donor-ion states are expected to be isolated from neighboring donor centers. In this case the spectral response observed from the photoexcitation of these states should closely resemble the electron photodetachment cross section from atomic H$^-$ ions,[6] when scaled according to the effective-mass theory. In Fig. 1(a) the experimental spectral response

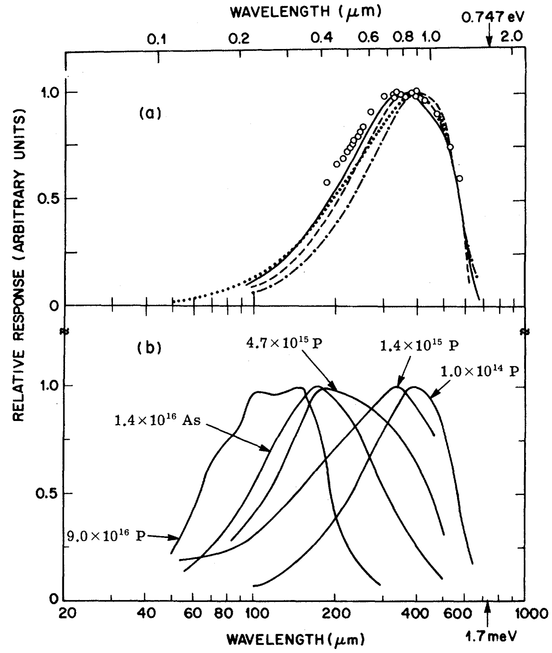

FIG. 1. (a) The relative spectral response of D^- centers in four lightly doped samples of n-type silicon [dash-dotted curve, 1.0×10^{14} cm^{-3} P; dashed curve, 1.4×10^{14} cm^{-3} P; solid curve, 5.0×10^{14} cm^{-3} As; dotted curve, 5.4×10^{14} cm^{-3} P] compared with the experimental photodetachment cross section of H$^-$ ions (open circles) measured by Smith and Burch (Ref. 6). The wavelength scales have been adjusted according to the ratio of m^*/ϵ^2 for this comparison and the peak values normalized to unity. Theoretical values for the binding energy of H$^-$ and D^- centers are noted. (b) The relative spectral responses of several samples are compared over the range of donor concentrations studied. The peak response is observed to shift to higher photon energies as the concentration of donors is increased.

of four lightly doped samples is compared with the experimental photodetachment cross section for atomic H$^-$, with the spectral maxima normalized to unity and the wavelength scales shifted by m^*/ϵ^2. The agreement is excellent and no significant difference is noted between the negative-ion states of P and As impurities.

At higher impurity concentrations the spectral response shifts towards shorter wavelengths and the shape of the response is found to vary with temperature.[7] The spectral response for several representative samples is shown in Fig. 1(b), measured at 2 K. As the concentration is increased, random impurity clusters form which have impurities spaced closely enough for the D^- wave functions to overlap. Electrons are bound more strongly to these donor groups than to isolated donors.[8] To display the concentration dependence of this effect I have chosen four arbitrary features from the spectra and noted the photon energy at which this feature occurred in each sample. The features are the signal maxima, the half-maxima on the short- and long-wavelength side of the maxima, and the quarter-maxima on the long-wavelength side. Figure 2 shows the photon energy at which the signal reaches each of these points as a function of the donor concentration. Solid lines have been drawn to trace the approximate average variation of these features. Based upon the shift by a factor of 2 in the photon energy corresponding to the peak signal at a donor concentration of 3×10^{15} cm^{-3} it is evident that the negative-donor-ion states have undergone a transformation in their character at this concentration.

If the upper Hubbard band has formed at this concentration then a range of localized energy states should be present for electrons to occupy between the band minimum and the mobility edge. The temperature dependence of the spectral response shape for samples doped slightly above the critical concentration verifies that a band of localized states exists. In Fig. 3 the spectral response is shown for a sample with a donor concentration of 8.5×10^{15} cm^{-3} for several temperatures in the range of 2 to 7 K. The long-wavelength response is observed to decrease rapidly as the temperature is initially raised above 2 K. This decrease occurs because the most weakly bound states within the band are thermally depopulated first. In the higher range of temperatures, however, the shape of the response has become fairly stable and only the signal intensity is observed to decrease. The responses shown here have been normalized to each other by observing the signal as a function of temperature from a submillimeter laser source at 118 μm. With this relatively intense source it is possible to follow the signal to higher temperatures. The signal as a function of inverse temperature is shown in Fig. 4 for data obtained in this way. At the highest temperatures the activation energy indicated is 7.6 meV. This value is consistent with the spectral shape seen at the highest temperatures in Fig. 3. For comparison, the temperature dependence of the signal from a sample doped be-

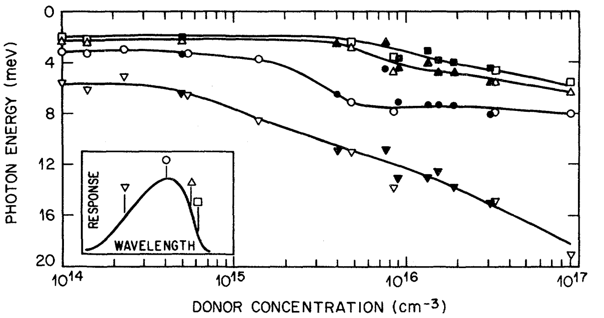

FIG. 2. Variations in the photon energy corresponding to selected features of the response from D^- centers as a function of the donor concentration. The features selected are noted in the inset. At about 3×10^{15} cm^{-3} the photon energy corresponding to the spectral response peak increases by about a factor of 2, corresponding to the formation of a band of states (upper Hubbard band). Phosphorous-doped samples are noted with open symbols and arsenic-doped samples with solid symbols.

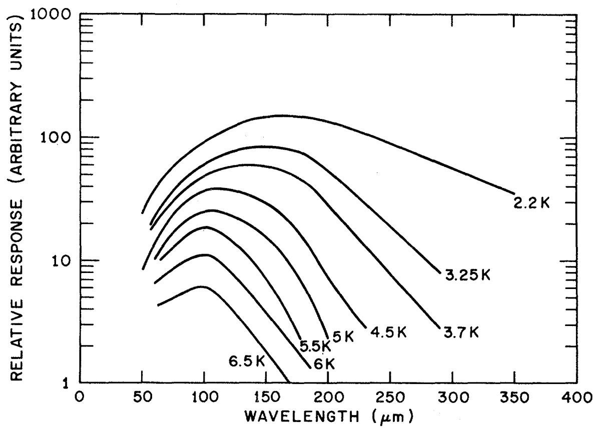

FIG. 3. Temperature dependence of the spectral response for a sample (8.5×10^{15} cm^{-3} P) above the transition concentration (3×10^{15} cm^{-3}). Localized states within the upper Hubbard band which are closest to the conduction band are the first states thermally depopulated as the temperature is raised.

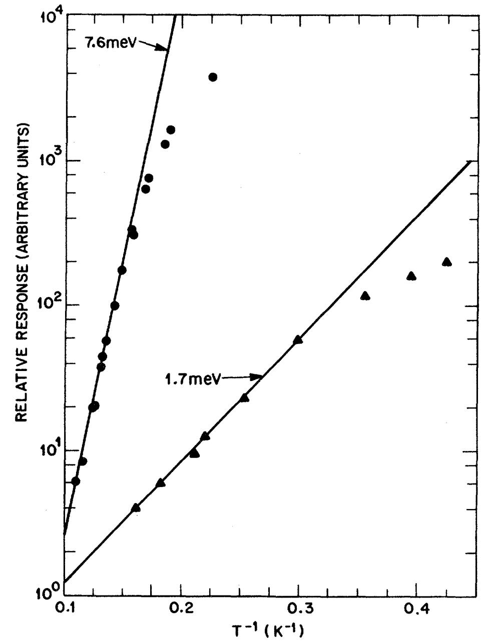

FIG. 4. The photoconductive response of two samples to a 118-μm laser source (photon energy 10.5 meV) as a function of inverse temperature. An activation energy corresponding to isolated D^- centers (1.7 meV) is observed for the sample having a donor concentration (P) of 5.4×10^{14} cm^{-3}. The activation energy for the more heavily doped sample corresponds to the lowest states within the upper Hubbard band which are seen to be 7.6 meV below the conduction band in this sample which has a donor concentration (P) of 8.5×10^{15} cm^{-3}.

low the critical concentration is also shown in Fig. 4. At a donor concentration of 5.4×10^{14} cm^{-3} the activation energy is observed to be 1.7 meV, consistent with the binding energy of isolated D^- centers.

From the concentration dependence of the spectral response it has also been possible to estimate the spatial extent of the D^- wave functions. This estimate is obtained on the basis of the signal strength at a wavelength of 400 μm as a function of donor concentration. 400 μm was chosen as the characteristic peak-response wavelength for isolated donors. The response signal at 400 μm will decrease relative to the peak signal when few isolated donors are present, and this decrease can be used to indicate the radius around a donor which must be free of other donors in order for it to be isolated. The donor separation necessary for isolation is found to be 250 Å, implying a donor-wave-function radius of 125 Å. As is known from impurity-hopping studies with neutral-donor centers, estimates of this type give wave-function radii about four times larger than the Bohr radius, since only the tails of the radial wave-functions need to overlap in order to begin influencing these states. Thus the radial extent of the wave function is more probably on the order of 30 Å. This value is about a factor of 1.5 greater than the wave function radius of the neutral-donor impurities calculated from the effective-mass theory. A comparison of the theoretical wave functions of H and H^- indicates that this estimate is very good, especially when it is taken into account that the D^- centers are described more accurately by the effective-mass theory than the neutral-donor centers. It should be noted in this context that the D^- wave functions are relatively compact compared with the neutral-impurity excited-state wave functions of comparable binding energy.

In summary I have shown that the upper Hubbard band which arises from overlapping states of the negative-donor ions in silicon doped with shallow impurities is formed at a donor concentration of 3×10^{15} cm^{-3}. Slightly above the critical concentration the bottom of this band is separated from the conduction band by 8 meV. The upper Hubbard band forms at a donor concentration about one and a half orders of magnitude lower than that necessary to form the lower Hubbard band, and three orders of magnitude lower concentration than that at which the metal-insulator transition is observed in this material. The negative-donor-ion states which form this band are described very well by the effective-mass theory, and within the experimental limits no chemical shift was observed between P and As impurities in their negative-ion states.

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Exact Self-Consistent Equilibria of Relativistic Electron Beams*

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Fully self-consistent and relativistically exact solutions for the equilibrium of a nonneutral, cold, relativistic, electron beam in a magnetized conducting pipe reveal that the beam is neither of uniform density nor a rigid rotor when total momenta and energy are uniform. The profiles are simple rational functions of the radius. Voltage-current-magnetization characteristics are obtained, showing a maximum current and a cutoff in magnetization for fixed injection voltage.

Equilibria of cold, nonneutral, relativistic, electron beams[1] have often been derived from a force-balance equation that represents one constraint on three distributions, typically those of density, rotation, and axial velocity. Equilibrium and stability analyses usually assume that the beam has a uniform density profile or rotates rigidly.[2] Such assumptions lead to equilibria constrained to have specific, nonuniform distributions of momenta and energy. The fully self-consistent, relativistically exact calculation below instead prescribes that all electrons are to have the same total (mechanical plus electromagnetic) momentum and energy. This is found to allow neither a rigid rotor nor a uniform density of the beam.[3]

An infinitely long, nonneutral, cold, relativistic electron beam propagates inside a circular conducting pipe, confined by an externally imposed axial magnetic field, B_0. The evacuated pipe has radius a, while the coaxial beam extends to radius r_0 where it has a sharp edge. The beam streams axially with mean velocity $v = \beta c$ and rotates about the axis, driven by the combined electric and magnetic fields. The fields expected in this system include a radial electric field $E_r(r)$ due to the nonneutralized charge, an azimuthal magnetic field $B_\varphi(r)$ from the streaming current, and an internally generated axial magnetic field $B_z(r)$ due to the rotation of the beam. These are derivable from an axisymmetric potential that has both axial and azimuthal components.

Space-time points are identified by a position four-vector x_α with imaginary temporal component $x_4 = ict$. The mean velocity four-vector of the beam, u_α, has nonzero components $u_3 = \gamma v$ and $u_4 = ic\gamma$, where $\gamma = (1-\beta^2)^{-1/2}$. The cross product with the axial unit vector is expressed by the antisymmetric tensor $Z_{\alpha\beta}$ whose nonzero components are $Z_{12} = -Z_{21} = -1$. The four-potential, $A_\alpha(x)$, that corresponds to the expected field pattern is

$$(e/m)A_\alpha(x) = p(r)u_\alpha + q(r)(\omega_c/2)Z_{\alpha\beta}x_\beta, \qquad (1)$$

where $(-e/m)$ is the ratio of electron charge to rest mass and $a_c = (e/m)B_0$ is the cyclotron frequency in the applied magnetic field. The two unknown radial profiles, $p(r)$ and $q(r)$, are to be determined self-consistently. In the absence of the beam, there is only the applied uniform magnetization, expressed by $p = 0$ and $q = 1$.

The four-potential satisfies the boundary conditions at the surface of the conducting pipe for any profiles p, q. It also satisfies the Lorentz gauge condition $\partial A_\alpha/\partial x_\alpha = 0$. The inhomogeneous wave equation is hence

$$\partial^2 A_\alpha/\partial x_\beta \partial x_\beta = -\mu_0 J_\alpha, \qquad (2)$$

which yields the four-current density, $J_\alpha(x)$, that accompanies and generates the potential,

$$-\mu_0 \frac{e}{m} J_\alpha = \frac{1}{r}\frac{d}{dr}\left(r\frac{dp}{dr}\right)u_\alpha + \frac{1}{r^3}\frac{d}{dr}\left(r^3\frac{dq}{dr}\right)\frac{\omega_c}{2}Z_{\alpha\beta}x_\beta. \qquad (3)$$