In the present investigation these difficulties were overcome and the agreement between the calculated and experimental values of μ, when the same scattering mechanisms were assumed throughout the full temperature range, was found to be quite satisfactory for epitaxial GaP films prepared from melts containing both Yb and free of this impurity. This could be regarded as an argument that gettering of impurities by ytterbium atoms occurred already in the melt. Otherwise the appearance of impurity complexes in epitaxial films would have unavoidably altered significantly the nature of the dependence $\mu(T)$, in conflict with our results.

We shall conclude by noting that the use of n-type GaP samples of higher quality and an allowance for the anisotropy of the scattering by acoustic phonons enabled us to refine the parameters of the intervalley scattering in these crystals. It was found that the experimental and calculated values of μ could be made to agree in the range $T \geq 300$ K only for an intervalley phonon with $T_{ph} = 150$ K. The constants representing the coupling of electrons to this intervalley phonon was found to be $D = 0.3 \cdot 10^9$ eV/cm.

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Nature of impurity states formed by transition metals (iron and europium) in amorphous hydrogenated silicon

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The problem of doping amorphous hydrogenated silicon a-Si:H has been attracting attention for a long time.[1] The main method for effective modification of electrical properties of a-Si:H is doping from the vapor phase.[2] We shall report the results of doping of a-Si:H with transition metals (iron and europium) by the sputtering method.

Our samples were formed by hf simultaneous sputtering of a single-crystal silicon target and a target made of iron (or europium) placed inside a mixture of helium, argon, and silane gases.[3] The substrate temperature was 250, 300, or 380°C. The concentration of metals was 0.1 at.% and the concentration of hydrogen was 15 at.%. The dark conductivity σ_d and the photoconductivity σ_{ph} were determined in a planar geometry. The photoconductivity was measured at 295 K during illumination with light of $4 \cdot 10^{17}$ photons$\cdot$cm$^{-2}\cdot$s^{-1} intensity and of 0.65 μm wavelength. The position of the optical absorption edge was determined at 295 K. Mössbauer spectra of ^{57}Fe and ^{151}Eu impurity atoms were determined at 294 and 80 K using ^{57}Co in palladium and $^{151}Sm_2O_3$ sources.

All undoped a-Si:H samples exhibited n-type conduction (and a negative room-temperature thermoelectric power of $\sim$200 μV/K), the optical width of the band gap was 1.70 ± 0.02 eV, and the temperature dependence of the electrical conductivity (Fig. 1) was linear when plotted using the coordinates log $\sigma - 1/T$ at temperatures in the range 100-500 K. Consequently, in this temperature range the process of conduction in undoped samples was due to electrons from delocalized states lying above the mobility edge E_c and the activation energy of the conduction process E_σ was defined as $E_\sigma = E_c - F$, where F is the Fermi level. The electrical conductivity and photoconductivity parameters depended strongly on the substrate temperature T_s (Table I) and it was found that changes in σ_d, σ_{ph}, and E_σ on increase in the substrate temperature T_s were of the same nature as for a-Si:H films prepared by decomposition of silane (see, for example, Ref. 2). Clearly, as in the case of a-Si:H formed from silane, an increase in T_s in the case of our films reduced the concentration of intrinsic defects and shifted the Fermi level toward E_c (for a sample prepared at $T_s = 380$°C the activation energy was $E_\sigma = 0.58$ eV).

Introduction of iron into a-Si:H altered the nature of the dependences: the values of σ_d and σ_{ph} decreased on increase in T_s, whereas E_σ rose with the substrate temperature (Fig. 1 and Table I), i.e., doping of a-Si:H with iron shifted the Fermi level toward the middle of the band gap. The doping effect was manifested particularly clearly in the case of films prepared at $T_s = 380$°C ($E_\sigma = 0.80$ eV). The thermoelectric power and the optical width of the band gap were not affected by doping.

The structure of the Mössbauer spectra ^{57}Fe depended on the substrate temperature. In the case of those samples which were prepared at $T \leq 300$°C the spectra consisted of quadrupole doublets (at 295 K the isomeric shift was $\delta = 0.20 \pm 0.02$ mm/s and the quadrupole splitting was $\Delta = 0.34 \pm$

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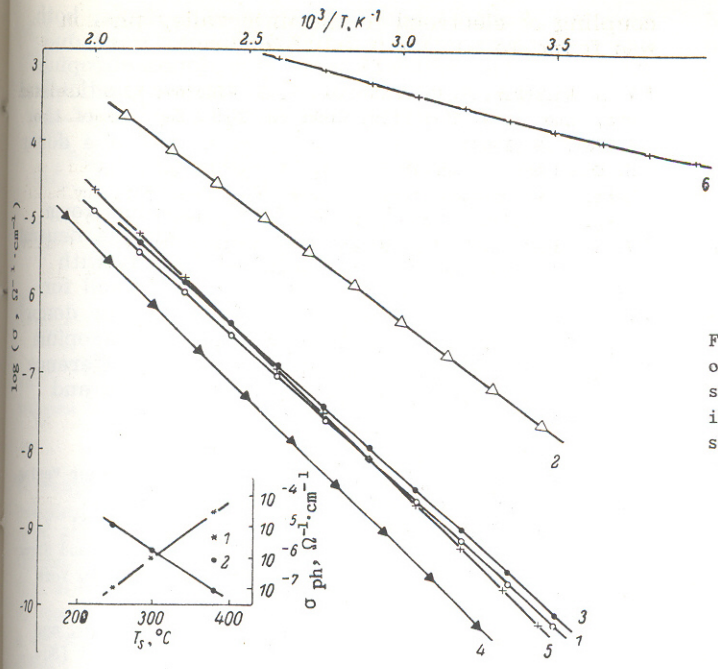

FIG. 1. Temperature dependences of the electrical conductivity of a-Si:H (1, 2), a-Si:H:Fe (3, 4), and a-Si:H:Eu (5, 6). Substrate temperature (°C): 1), 3), 5) 250; 2), 4), 6) 380. The inset shows the dependence of the photoconductivity on the substrate temperature T_S for a-Si:H (1) and a-Si:H:Fe (2).

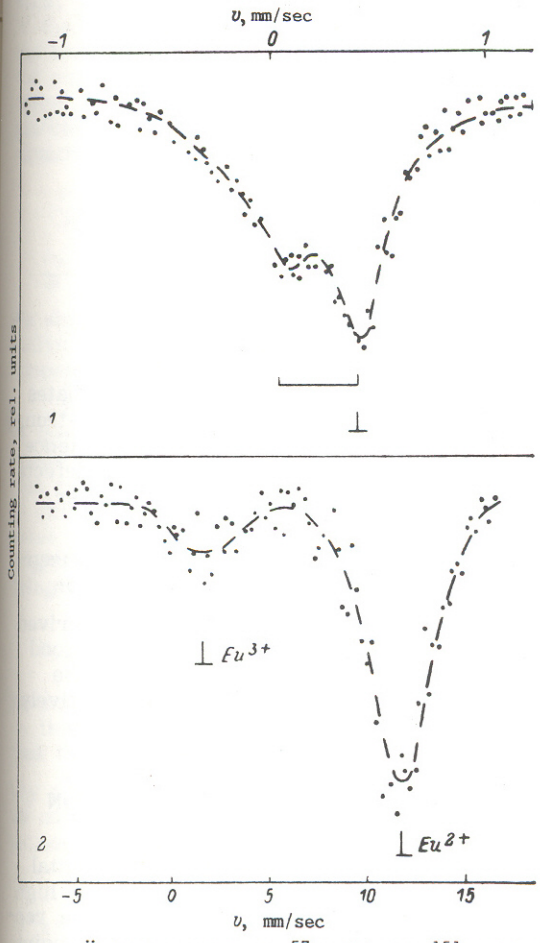

FIG. 2. Mössbauer spectra of ^{57}Fe (1) and ^{151}Eu (2) impurity atoms in a-Si:H deposited on a substrate kept at T_S = 380°C. In the case of the spectrum of ^{57}Fe the analysis into a quadrupole doublet and a single line is shown.

0.03 mm/s). According to Ref. 3, this spectrum represented iron–vacancy associates. In the case of the samples prepared at T_S = 380°C this doublet was supplemented by an additional singlet representing isolated iron atoms in the Fe^{3+} state (δ = 0.35 mm/s relative to α-Fe; Fig. 2a). Clearly, the iron centers were responsible for the change in the electrical conductivity of doped a-Si:H. At temperatures $T_S \leq 300$°C the vacancy concentration was higher than that of iron and practically all the impurity atoms were bound forming electrically inactive iron–vacancy complexes. At T_S = 380°C the vacancy concentration fell and a considerable fraction of iron atoms [intensity of the Mössbauer spectrum indicated that this fraction was $(1\text{-}2)\cdot10^{19}$ cm^{-3}] was in an electrically active state.

The influence of the iron impurity on electrical properties of a-Si:H was due to the fact that isolated iron atoms formed a band of acceptor levels in the mobility gap. The Fe^{3+} singlet in the Mössbauer spectrum was due to the neutral state of the iron acceptor centers. The absence of the Fe^{2+} line, which would correspond to the ionized state of center, indicated a low occupancy of the acceptor band, i.e., that the Fermi level was in the lower part of this band. Consequently, the density of states in the gap between the position of F in the doped and undoped samples was low compared with the acceptor concentration. The Fermi level in the iron-doped samples formed at T_S = 380°C was clearly pinned to the acceptor band of iron and the value E_σ = 0.80 eV indicated the position of

TABLE I. Parameters of electrical conductivity of a-Si:H

Composition	T_s, °C	E_σ, eV	$\sigma_{0\sigma}$, $\Omega^{-1}\cdot cm^{-1}$	σ_{295}, $\Omega^{-1}\cdot cm^{-1}$
a-Si:H	380	0.58	280	$3.4\cdot10^{-8}$
a-Si:H:Fe	380	0.80	320	$1.9\cdot10^{-11}$
a-Si:H:Eu	380	0.20	0.56	$5.0\cdot10^{-4}$
a-Si:H	300	0.71	1300	$6.3\cdot10^{-10}$
a-Si:H:Fe	300	0.69	89	$9.5\cdot10^{-11}$
a-Si:H:Eu	300	0.56	320	$5.0\cdot10^{-7}$
a-Si:H	250	0.70	180	$1.5\cdot10^{-10}$
a-Si:H:Fe	250	0.69	200	$1.9\cdot10^{-10}$
a-Si:H:Eu	250	0.68	1300	$1.0\cdot10^{-9}$

this band relative to E_C. However, this value could be an overestimate for $E_C - E_{Fe}$ (E_{Fe} is the position of the Fermi band), because the iron centers were mainly neutral and F could be pinned below the iron band. Clearly, the iron centers also have a recombination function reducing the photoconductivity of the doped material (Fig. 1).

In contrast to iron, the impurity atoms of europium increased the electrical conductivity of a-Si:H, but the effect of doping increased (as in the case of iron) on increase of T_S (Fig. 1 and Table I). The thermoelectric power and the optical width of the band gap were not affected by doping. This indicated that the introduction of europium into a-Si:H shifted the Fermi level toward E_C (for a sample formed at T_S = 380°C the activation energy was E_σ = 0.25 eV). The influence of the europium impurity could be explained by the formation, within the mobility gap of a-Si:H, of a band of donor levels in which electrons occupied the lower vacant states and lifted the Fermi level. According to this model the doping efficiency should increase on reduction in the concentration of intrinsic defects, as manifested by the dependence of F on the substrate temperature in the case of europium-doped samples (Table I).

The Mössbauer spectra of ^{151}Eu in a-Si:H (Fig. 2b) consisted of two lines representing Eu^{2+} (δ = −11.7 mm/s) and Eu^{3+} (δ = −1.7 mm/s, both shifts relative to Eu_2O_3). These lines were due to neutral and ionized states of a donor europium center, respectively. Two 6s electrons participated in the formation of chemical bonds and one of the 4f electrons of europium played the role of a donor electron.

We thus found that iron and europium form electrically active centers in a-Si:H and the neutral state of these centers corresponds to ions with a half-filled $3d^5$ shell for iron and $4f^7$ shell for europium. The different nature (acceptor or donor) of the electrical activity of the iron and europium centers can clearly be attributed to the difference between the properties of the half-filled 3d and 4f shells of these elements.

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Mechanism of boron diffusion in silicon carbide

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Diffusion of boron is one of the main methods used in the formation of p-n junctions in silicon carbide and it has been the subject of many experimental investigations.[1-6] These investigations have been established certain anomalous features of the diffusion process which have not yet been explained adequately. The most important anomaly is a nonlocal dependence of the diffusion coefficient of boron on the concentration of this impurity: the rate of boron diffusion is governed not only by the concentration c_B and its gradient, but it also depends strongly on the boron concentration on the surface of a crystal c_B^S: $D_B = f(c_B, c_B^S)$. The dependence of the diffusion coefficient on c_B^S is so strong that the profiles of the concentration of boron established by diffusion change radically when c_B^S is altered. It is suggested in Refs. 5 and 6 that these anomalies are associated with the existence of a whole series of various boron associates, of which the most mobile is a B_C–V_C complex, and also due to generation of excess vacancies because of the donor–acceptor interaction.

We shalls how that the observed phenomena can also be explained in a natural manner by an impurity diffusion model invoking mobile impurity–defect associates of one type. We shall postulate that boron can migrate in the lattice of SiC only in the form of such associates. In the course of diffusion in the bulk of a crystal these associates break up and the bulk of a crystal becomes strongly enriched with intrinsic defects. The consequence of such pumping of nonequilbrium intrinsic defects is an increase in the probability of the transfer of boron to a mobile associate.

An analytic expression for a nonlocal concentration-dependent diffusion coefficient of boron migrating in SiC, $D_B + f(c_B, c_B^S)$, will be derived and boron distribution profiles which are in good agreement with the experimental results will be calculated. The formal description is qualitatively similar to that discussed earlier for silicon by Ioshida [7] and by Morehead and Lever.[8]

1. FORMAL DESCRIPTION OF THE DIFFUSION PROCESS

There are at present no direct experimental data on the diffusion-mobile state of boron at high temperatures. We shall assume that this state represents an associate of a boron atom with a point lattice defect The simplest model of formation of such an associate, which we shall consider later, is described by the reaction equation

$$B + D = A, \quad c_B c_D = c_A k(T), \tag{1}$$

where B, D, and A represent boron, a point defect, and an associate; c_B, c_D, and c_A are the

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