Non-Lorentzian Noise at Semiconductor Interfaces

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Electrical noise at silicon grain boundaries deviates significantly from Lorentzian behavior. The noise shows a $1/f$ dependence over a wide frequency range. We present a new model to explain this behavior quantitatively. Our model is based on generation and recombination of charge carriers at interface states and explicitly takes into account inhomogeneities within the boundary plane. Such inhomogeneities generally cause deviations from Lorentzian spectra. The quantitative analysis allows us to characterize these interface states.

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An exponential time behavior often suffices to describe relaxation processes of ideal physical systems towards equilibrium. An exponential decay law of the form $\exp(-t/\tau)$ with time constant τ and time t corresponds to a Lorentz spectrum $S_U^{\text{Lorentz}}(f)$ at frequency f in the noise properties of the system. The noise reflects the stochastic fluctuations of the system around steady-state values (for example, fluctuations of voltage U in a constant-current experiment)[1]:

$$S_U^{\text{Lorentz}}(f) \sim 1/[1+(2\pi f\tau)^2]. \quad (1)$$

In real systems, however, one often encounters *nonexponential* decay laws.[2] This feature finds its counterpart in the observation of *non-Lorentzian* noise spectra. The most prominent non-Lorentzian noise is the so-called $1/f^n$ noise, where for the noise power density S a dependence $S \sim 1/f^n$ with $n \approx 1$ is observed over a wide frequency range.[1]

There is no generally accepted theory for the explanation of $1/f^n$ noise in the electrical conductance of semiconductors.[1,3] Two schools of thought can be discerned. The main controversy is whether the $1/f^n$ noise is due to fluctuations in the number or in the mobility of free charge carriers. One school employs an empirical equation for a so-called α noise, first suggested by Hooge[4] assuming mobility fluctuations. The other school ascribes $1/f^n$ noise to number fluctuations and to a distribution of time constants τ, originating from a superposition of Lorentzian generation and recombination processes at traps. This model was first discussed by McWhorter[5] for the description of noise from metal-oxide-semiconductor interfaces. Nearly all papers on $1/f^n$ noise restricted themselves to perfectly ordered crystals or, in the case of interfaces, to a perfect order within the boundary plane. Spatial periodicity of the lattice and consequently spatial homogeneity of the band edges were tacitly assumed.

In this Letter we introduce a new concept into the description of $1/f^n$ noise at semiconductor interfaces. Our model is based on the fundamental insight that the localization of carriers in interface states per se leads to a distribution of time constants τ: The random spatial distribution of charged interface states within the boundary plane results in a spatial modulation of the band edges by electrostatic forces. These potential fluctuations cause a *spatial* distribution of time constants for generation and recombination processes. This dispersion of time constants leads to a transition from Lorentzian to $1/f^n$-like noise.

The significance of potential fluctuations has been discussed for metal-oxide-semiconductor interfaces[6] and for grain boundaries[7] and should also be found at other interfaces such as Schottky contacts or heterojunctions. Here we give the first *quantitative* analysis of the effect of potential fluctuations on the noise properties of semiconductor junctions. We restrict ourselves to silicon grain boundaries because the electronic properties of these interfaces are exclusively controlled by interface states and their spatial distribution.[7,8]

The grain boundaries are obtained from silicon bicrystals that are Czochralski grown by a double-seed technique.[9] The crystallographic parameters of the grain boundary are adjusted by the relative orientation of the two seeds. The samples discussed in this Letter are cut from a p-type Si bicrystal with a boron concentration of $N_A = 1\times10^{15}$ cm^{-3}. The grains are tilted around a [110] direction by an angle of 7.8°.

Figure 1 shows the band diagram at the grain boundary. The crystallographic misfit at the boundary induces donorlike and acceptorlike interface states. They interact with the conduction and valence bands via capture and emission of electrons and holes. The positive interface charge and the interaction with the valence band prevail for p-type silicon.[7,8] This positive interface charge results in a negatively charged depletion region around the grain boundary and a potential barrier height $e\phi$ that hinders the current transport by free holes. Within the model of thermionic emission[8] the current density j_{th} across the boundary under the application of bias voltage U is given by

$$j_{\text{th}} = A^*T^2\exp[-e(\zeta+\phi)/kT] \times[1-\exp(-eU/kT)], \quad (2)$$

where A^* is the Richardson constant, kT/e is the ther-

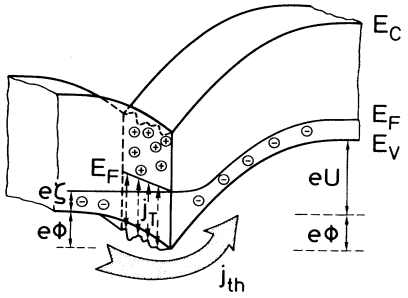

FIG. 1. Band diagram at the grain boundary in p-type silicon. Only donorlike interface states are drawn for simplicity. The positive interface charge is compensated by negative acceptor ions within the space-charge region. The application of a voltage U results in a thermally emitted current j_{th} over the barrier $e\phi$. The current j_T represents the capture and emission of holes by the deep interface states. The spatial distribution of these traps leads to potential fluctuations.

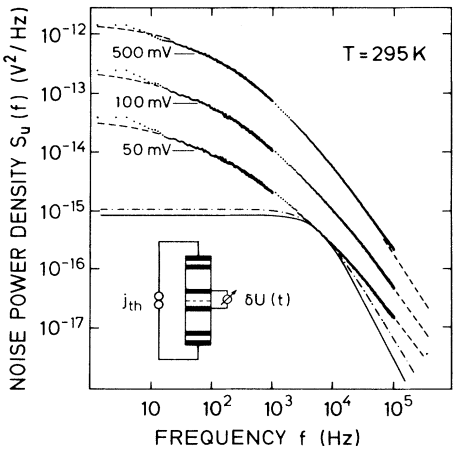

FIG. 2. Noise spectra of a grain boundary (dashed line in inset) in a silicon bicrystal for various voltage drops. Shot noise is subtracted. The full line indicates Lorentzian noise after Eq. (1), as expected for monoenergetic interface states. The dash-dotted line is for an interface-state continuum after Eq. (4). The dashed lines originate from the potential-fluctuation model, Eq. (5), under the consideration of the spatial distribution of interface defects. Our contact configuration allows measurements across the boundary as well as in the single-crystalline grains.

mal voltage, and $e\zeta$ is the Fermi level within the grains that is measured by the Hall effect.

In our experiments, we keep the current j_{th} constant. The stochastic capture and emission of holes at the interface result in stochastic fluctuations of the trapped positive interface charge Q. Overall charge neutrality and the experimental condition of a constant current then cause stochastic fluctuations of the width of the compensating negatively charged space-charge region and of a barrier height $e\phi$. This mechanism results in voltage fluctuations $\delta U(t)$.

We amplify, filter, and then digitize $\delta U(t)$ in analog-to-digital converters, and perform a Fourier transformation of the digitized signal with the help of an array processor. The square of the Fourier components is proportional to the voltage-noise power density $S_U(f)$. Amplifier noise is suppressed by a cross-correlation technique.[10] The computation speed of the array processor enables us to perform precise measurements in a reasonable time. The measurements presented in this Letter are obtained from a compilation of two spectra, each containing 1024 points spaced by 1.25 and 125 Hz, respectively. Up to 19 000 samplings have been averaged in about 40 min.

Figure 2 shows the experimental results. The measured noise exceeds the noise of the adjacent grains as well as the shot noise of the grain boundary by orders of magnitude. The spectra vary smoothly with frequency and show a $1/f^n$ behavior over a wide frequency range.

We explain the measured noise spectra by the mechanism described above; detailed numerical analysis will be discussed elsewhere.[11] Our model describes the stochastic capture and emission current j_T between majority carriers and traps with the help of Shockley-Read-Hall statistics.[12] The analysis then finally yields the noise power density $S_Q(f)$ for the fluctuations of the trapped interface charge Q. The measured noise $S_U(f)$ of Fig. 2 is proportional to $S_Q(f)$ (Ref. 11):

$$S_U(f) = S_Q(f)/C_R^2. \tag{3}$$

Here C_R is the high-frequency capacitance of the right-hand-side reverse-biased space-charge region.

First, we analyze the applicability of a Lorentzian behavior as described by Eq. (1) which is expected for a monoenergetic interface state.[1] The comparison in Fig. 2 shows the poor agreement of such a model with the measured curves. Next, we consider an energy continuum of interface states that is observed at silicon grain boundaries.[7] Such a continuum leads to a frequency dependence of $S_U^{\rm cont}(f)$ that is only slightly different from the Lorentzian form of Eq. (1), since only states within a few times kT around the Fermi level E_F contribute to the noise[11]:

$$S_U^{\rm cont}(f) = \frac{2kTe^2N_{SS}}{C_R^2A}\,\frac{\ln[1+(2\pi f\tau_p)^2]}{(2\pi f)^2\tau_p}. \tag{4}$$

Here N_{SS} is the areal density of interface states at the Fermi level E_F, and A is the grain boundary area. The time constant τ_p is given by $\tau_p(\upsilon p S_p)^{-1}$, where $p = p_G \exp(-e\phi/kT)$ is the concentration of holes at the grain boundary, p_G their concentration within the grains, υ their thermal velocity, and S_p the capture

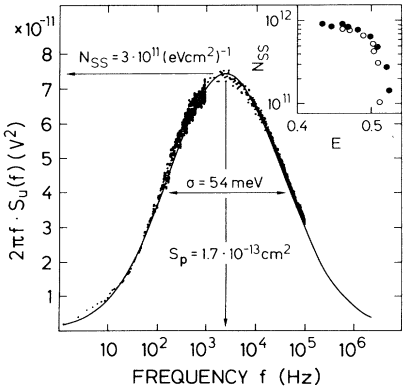

FIG. 3. The product of spectral density $S_U(f)$ and frequency $2\pi f$ for the 100-mV spectrum of Fig. 2. The full line is obtained from the potential-fluctuation model with use of the shown values for the density of states N_{SS}, the capture cross section S_p, and the standard deviation of the potential fluctuations σ. The inset shows the density of states N_{SS} [in (eV cm^2)$^{-1}$] vs band-gap energy E (in electronvolts) as obtained from measurements at different voltage drops and temperatures. The zero energy point is at the valence-band edge at the interface. The full circles are obtained from noise measurements; the open circles are from admittance spectroscopy.

cross section of the interface states for holes. The spectral density $S_U^{\text{cont}}(f)$, as obtained from Eq. (4), also agrees poorly with the measured curves as shown in Fig. 2.

The discrepancy is resolved by accounting explicitly for the localized nature of the trapped charge Q. This localization leads to a random spatial variation of the barrier $e\phi$ along the interface plane, as sketched by the ragged lines in Fig. 1. The distribution $P(\phi)$ of barriers is in a first approximation a Gaussian with mean $\bar{\phi}$ and standard deviation σ. We consider the contribution to the noise spectrum due to capture and emission of charge carriers which cross the boundary at different barrier heights ϕ as independent. The resulting noise spectrum is obtained by multiplication of the spectrum of Eq. (4) by the distribution $P(\phi)$ and integration over all barrier heights[11]:

$$S_U^{\text{PF}}(f) := \int_{-\infty}^{+\infty} P(\phi) S_U^{\text{cont}}(f)\, d(\phi - \bar{\phi}). \qquad (5)$$

The resultant spectral density S_U^{PF} agrees excellently with the measured spectra as demonstrated in Fig. 2.

The integration in Eq. (5) cannot be done analytically, but Simonne[13] proposed a procedure that allows a straightforward evaluation of the measurements by taking into account only two points of the measured spectrum. This is conveniently done by multiplication of the measured spectra $S_U(f)$ with the frequency $2\pi f$. This product, $2\pi f S_U(f)$, shows a broad maximum as demonstrated in Fig. 3 for the 100-mV spectrum of Fig. 2. The height of the maximum is proportional to the density of interface states N_{SS}; the frequency where the maximum occurs is proportional to the capture cross section S_p; the width of the curve is a measure for the standard deviation σ of the distribution function of the potentials.

The Fermi level E_F can be swept through the forbidden gap by variation of the bias voltage U and temperature T. The resultant energy dependence of the density of interface states $N_{SS}(E)$ agrees excellently with $N_{SS}(E)$ as obtained from admittance spectroscopy,[7] as shown in the inset of Fig. 3. Excellent agreement is also obtained for the capture cross section S_p and the standard deviation σ of the potential fluctuations.[11] The capture cross section S_p varies from 2×10^{-14} cm^2 to 2×10^{-13} cm^2 and depends on temperature T. The standard deviation σ has a value of 50 ± 5 meV independent of temperature and bias voltage. This value is to be compared with a typical mean barrier height of $\bar{\phi} \simeq 300$ meV.

In conclusion, we have shown that an idealized model for semiconductor interfaces which tacitly assumes spatial homogeneity of the band edges fails to explain the noise properties of these interfaces. We have demonstrated that the localization of charge in interface states by itself locally distorts the potential. The potential fluctuations appreciably influence the transport properties of the material. Especially, the localization per se leads naturally to a distribution of time constants τ and thus gives an explanation for the transition from Lorentzian noise to $1/f^n$ noise. The quantitative evaluation of the noise measurements within this potential-fluctuation model represents in addition a new method for the characterization of semiconductor grain boundaries.

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