

Size effect on current fluctuations in thin metal films: Monte Carlo approach

O. M. Bulashenko, O. V. Kochelap, and V. A. Kochelap

Department of Theoretical Physics, Institute of Semiconductors, Ukrainian Academy of Sciences, Kiev, 252650, Ukraine

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Current fluctuations associated with the classical size effect, for which the mean free path of the carriers λ is comparable to, or greater than, the film thickness d , have been investigated. The Monte Carlo approach has been extended into the Knudsen regime of electron transport. Using this method, the autocorrelation function and the spectral density of the fluctuations depending on two parameters (the ratio $\gamma = \lambda/d$ and the surface specularity p) have been calculated. A procedure to generate the angle of diffuse electron scattering at the surface is described for both the Fuchs and the Soffer boundary conditions. It is demonstrated for both models that, with increasing γ and with decreasing p , the low-frequency noise is suppressed, with a redistribution toward higher frequencies. In such a case, the autocorrelation function is not exponential and the corresponding spectral density of the fluctuations is no longer Lorentzian.

I. INTRODUCTION

Thin metal films have been studied for several decades and have remained interesting topics for various physical investigations. Films of a few micrometers in thickness are often used as electrical interconnections in microchips, multilayer hybrid packages designed for very-large-scale-integrated circuits, and so on.^{1,2} In physical studies and applications, both the conductivity and the current noise of the films are of primary interest because an understanding of these characteristics can ultimately result in the specification of optimum operating conditions, in part to minimize voltage drops along the interconnects and to maximize the integrity of high-speed signals propagating through them or to improve the signal-to-noise ratio.

It is known that when the mean free path of the carriers becomes comparable to, or greater than, the smallest dimension of the specimen, the conductivity becomes dependent on the size of the sample.^{3,4} A quantitative model of this so-called classical size effect has been proposed by Fuchs.⁵ A great number of papers dealing with this problem have been published. In most of them *only resistivity* of the thin films or wires as dependent on size, temperature, and surface reflection conditions was examined both theoretically and experimentally (see Refs. 3 and 4).

It is obvious that the *current noise*, being not less an important characteristic of transport phenomena, becomes dependent on the sample size too. In this paper, we study changes in the current fluctuations due to electron scattering at the boundaries, i.e., under size-effect conditions.

We consider the thermal current noise associated with velocity fluctuations of electrons under the above-mentioned conditions.

The autocorrelation function and the noise spectral density of the random process can be estimated by use of the Monte Carlo method, which is the most suitable one for this purpose, because it is easy to connect the fluctua-

tive variables with the microscopic motion of the charge carriers. Monte Carlo simulation of this kind of noise but without regard for the finite size of the sample has been performed by various investigators for some materials: InP,^{6,7} *p*-type Ge,⁸ Si,⁹⁻¹² GaAs,^{7,9,12-14} InSb,¹⁵ $\text{In}_x\text{Ga}_{1-x}\text{As}$.¹⁶

The aim of the paper is to reveal the main features of changes in the autocorrelation function and the noise spectral density of the current fluctuations in the thin metal film by decreasing its thickness and varying its surface roughness.

The paper is organized as follows. In Sec. II we define the physical model and introduce the main characteristics of the noise which are to be calculated. In Sec. III the particularities of the Monte Carlo method used are described, with special attention being paid to boundary reflection conditions. Two different types of boundary conditions are considered: (a) according to the Fuchs model⁵ and (b) according to Soffer.¹⁷ The results obtained are discussed in Sec. IV. A comparison with the theoretical results of another author is made for some cases. Section V draws the main conclusions of this work.

II. THE PHYSICAL MODEL

We consider a monocrystalline metal film under steady electric field applied along its surfaces. The thickness of the film d is comparable with the mean free path of the electrons λ . It is assumed that the transverse field can be neglected, owing to the Debye screening length being much less than λ . The electric field is then uniform across the sample.

The size effect occurs normally at low temperatures, when the mean free path is rather large. Under this condition the electron properties are entirely determined by the most energetic electrons near the Fermi surface, all moving with the same velocity V_F in arbitrary directions. For simplicity it is assumed that the electron Fermi surface is spherically symmetric and the bulk mean free path

is isotropic. The average time between collisions in the bulk τ (due to impurities or phonons) is constant and equal to λ/V_F . Each mechanism of the bulk scattering is assumed to be elastic, entirely chaotic, and independent of the velocity direction before collision.

Besides the scattering in the bulk, the electrons are scattered at the boundaries. The latter scattering is considered to be elastic and characterized by a parameter p , representing the fraction of specularly reflected electrons; for fully specular scattering $p=1$ and in the opposite case of fully diffuse scattering $p=0$. The parameter p has been introduced by Fuchs and in his model it was independent of the angle of electron incidence. The Fuchs model, being the most simple, is frequently used by many authors. More recently Ziman¹⁸ has determined the effect of geometrical roughness of the surface on the specularity parameter at normal incidence. Soffer¹⁷ has extended the method of Ziman to include oblique incidence and modified it to satisfy the flux-conservation requirement. As a result, the diffuse surface scattering was found to be anisotropic in the general case and the angular dependence of the specular parameter p was obtained in the form¹⁹

$$p(\theta) = e^{-(4\pi R \cos\theta)^2} . \quad (1)$$

Here, θ is the angle of the incidence with respect to the normal, R is the ratio of the surface rms height deviation h to the de Broglie wavelength of electrons λ_0 . The parameter R will be called here as a roughness coefficient. To study the current fluctuations we consider both the Fuchs model and the Soffer model. An appropriate comparison of the results will be made later in the paper.

Thus there are only two dimensionless parameters in our problem: (1) $\gamma = \lambda/d = V_F\tau/d$, that is the ratio of the mean free path to the film thickness, (2) the specularity parameter of the surface p (in the case of the Fuchs model) or the roughness coefficient R (in the case of the Soffer model).

By neglecting interaction between electrons the noise spectral density of the current fluctuations $S_I(\omega)$ can be assumed to be proportional to that of the velocity fluctuations $S_v(\omega)$:⁶

$$S_I(\omega) = \frac{e^2 n A}{L} S_v(\omega) . \quad (2)$$

Here, e is the electron charge, A is the cross-sectional area of the sample, L its length, n is the electron density, and ω is the frequency. Hence it is quite enough to calculate $S_v(\omega)$ to obtain the current noise.

According to the Wiener-Kintchine theorem, the velocity fluctuation spectrum $S_v(\omega)$ is given by the Fourier transform of the velocity autocorrelation function $C_v(t)$:

$$S_v(\omega) = 4 \int_0^\infty C_v(t) \cos(\omega t) dt . \quad (3)$$

The autocorrelation function $C_v(t)$ is defined as

$$C_v(t) = \langle \delta V(t') \delta V(t'+t) \rangle , \quad (4)$$

where angle brackets indicate the averaging over the electron ensemble, t is the lag time, $\delta V(t) = V(t) - \langle V \rangle$ is the

velocity fluctuation around the average value $\langle V \rangle$. The function $C_v(t)$ is independent of time t' for stationary process, which we study.

The main problem now is to evaluate $C_v(t)$ and $S_v(\omega)$ using Eqs. (3) and (4) as dependent on parameters γ and p .

III. MONTE CARLO SIMULATION

Electron drift velocity in metals is usually much less than V_F . This means that the velocity increment due to the electric field action during free flight between collisions is small. Hence to find the fluctuations of velocity around its average value, it suffices to consider the fluctuations of velocity itself, the average value being neglected.

Because of stationarity and ergodicity of the random process, we can use the time average instead of the ensemble average and the one-particle Monte Carlo technique²⁰ is to be applied. The path of a single electron is followed by computer simulation. The electron is considered to move quasiclassically during periods of free flight. Since the probability of free flight of the electron without any collision during the time t_r is proportional to $\exp(-t_r/\tau)$, the time t_r is determined from²⁰ $t_r = -\tau \ln r$, where r is a random number uniformly distributed between 0 and 1. The free flights are interspersed with scattering events occurring in the bulk or at the film boundary. If the electron does not collide with the surface for the time t_r , the bulk scattering occurs at the end of the flight, the angle after collision being taken as random with the equal probability. When the surface scattering takes place, one of the two possible reflections is chosen to occur. The choice is realized by generating a random number $r \in [0, 1]$ and after comparing it with the value of p , which is given in the Fuchs model or estimated by Eq. (1) in the model of Soffer. The specular reflection is adopted when $r < p$, and the diffuse one is taken in the opposite case. According to the choice the reflection angle is defined, the next free flight is generated, and the procedure is repeated.

Within the described model the angle of reflection is equal to that of incidence in the case of specular surface scattering. As for the diffuse scattering this relation is not satisfied and the electron velocity is randomized. In order to define the diffuse reflection angle θ_r , one has to take into account that the electron flow toward the surface must be equal to the flow backward. This flux-conservation requirement provides the uniform electron density across the film and quasineutrality condition to be satisfied.

Let us consider two different models of the surface scattering in details.

(a) *The Fuchs boundary condition.* In accordance with the flux-conservation requirement the electron leaves the surface in the direction Ω inside the elementary solid angle $d\Omega$ with the probability²¹ $\cos\theta d\Omega/\pi$. The random value θ_r may be related to the uniformly distributed random number r by

$$r = \frac{1}{\pi} \int_0^{\theta_r} \cos\theta \sin\theta d\theta \int_0^{2\pi} d\varphi. \quad (5)$$

From here one can obtain the formula to generate the random angle of diffuse electron scattering at the surface:

$$\cos\theta_r = \sqrt{r}. \quad (6)$$

(b) *The Soffer boundary condition.* The number of electrons specularly reflected in direction θ within $d\theta$ is proportional to $p(\theta) \cos\theta \sin\theta d\theta$. In view of flow conservation the number of the electrons diffusely reflected $\propto [1-p(\theta)] \cos\theta \sin\theta d\theta$, since the number of incident electrons within the same angle interval is proportional to $\cos\theta \sin\theta d\theta$.

By using Eq. (1) the probability for the diffuse scattering angle can be written as

$$\begin{aligned} W(\theta)d\theta &\propto [1 - e^{-(4\pi R \cos\theta)^2}] \cos\theta \sin\theta d\theta \\ &\propto [1 - e^{-(4\pi R)^2 \xi}] d\xi. \end{aligned} \quad (7)$$

Here, $\xi = \cos^2\theta$. This distribution may be related to the uniformly distributed random number r by

$$r = \frac{\int_0^{\xi_r} (1 - e^{-(4\pi R)^2 \xi}) d\xi}{1 - e^{-(4\pi R)^2}}. \quad (8)$$

The integral (8) one can evaluate analytically but the resulting equation is not possible to solve with respect to ξ_r . That is why we used the rejection technique²⁰ to generate the random value ξ_r and then θ_r was taken from

$$\cos\theta_r = \sqrt{\xi_r}. \quad (9)$$

Let us compare the resulting formulas for both models. In the limit of large surface roughness R ($\lambda_0 \lesssim h$) the specular parameter p becomes equal to zero, the exponent in Eq. (8) is much less than 1, and ξ_r becomes equal to r . Thus Eqs. (6) and (9) are equivalent. In the limit of small surface roughness ($\lambda_0 \gg h$) $p \approx 1$ and the specular reflection is dominated. Hence for smooth and rough cases both the Fuchs and the Soffer boundary conditions are identical. But for an intermediate case this is not so. In the Soffer model at grazing incidence the diffuse flux vanishes and the specular scattering dominates for arbitrary roughness.

Following the electron path the values of longitudinal velocity are stored in the computer after every time interval Δt . The simulation lasts until about 10^5 collisions, which randomize the electron velocity, occur. The obtained time series $V(t_i)$ defined in N points is used to estimate the autocorrelation function:

$$\begin{aligned} C_v(t_j) &= \lim_{N \rightarrow \infty} \left[\frac{1}{N} \sum_{i=1}^{N-j} V(t_i) V(t_i + j \Delta t) \right], \\ &j=0, 1, \dots, N_T. \end{aligned} \quad (10)$$

The equation gives $(N_T + 1)$ values of the autocorrelation function at time moments $t_j = j \Delta t$. The function $S_v(\omega)$ is calculated from (3) by using the trapezoidal formula.

IV. RESULTS AND DISCUSSION

Before studying the noise characteristics, some tests of the Monte Carlo program code have been made. The size effect may be associated with the Knudsen flow of electrons as a rarefied gas, where most of their collisions are with boundaries. The parameter γ is equivalent to the Knudsen number N_{Kn} , the latter being equal to the ratio of the molecular mean free path to a characteristic linear dimension. In such a consideration, using the well-known formula for molecular collision frequency with the surface, one can find the ratio of the electron collision frequency with the boundaries to that in the bulk:

$$\frac{\nu_b}{\nu_v} = \frac{\frac{1}{4} n V_F S_b}{\frac{1}{\tau} n V} = \frac{\lambda S_b}{4V} = \frac{\lambda}{2d} = \frac{1}{2} \gamma. \quad (11)$$

Here, S_b is the area of the surface on which the electrons are scattered, V is the sample volume. Hence the collision frequency ratio determined during Monte Carlo simulation may be used as a proof of the algorithm correctness. This ratio calculated in our work coincides with the predicted value with discrepancy less than 1% for any γ and p , indicating that the Monte Carlo procedure is correct. Moreover the uniformity of the electron density distribution across the film was verified.

Let us now consider the results obtained within the *Fuchs model*. The functions $C_v(t)$ and $S_v(\omega)$ (normalized to $\frac{1}{3} V_F^2$ and $\frac{4}{3} V_F^2 \tau$, respectively) are shown in Figs. 1 and 2. For fully diffuse boundary scattering ($p=0$) and for different γ the curves $C_v(t)$ are presented in Fig. 1(a). The value of $\gamma=0$ corresponds to the case $\lambda \ll d$, when the film thickness is infinite and the surface does not effect on the electron scattering. It has been pointed out⁷ that, if (i) the probability of electron motion without collisions is exponential and if (ii) each scattering event entirely randomizes electron velocity, the autocorrelation function has to be exponential with a time decay constant equal to τ , i.e., the average time between collisions. In our model conditions (i) and (ii) are satisfied. The function $C_v(t)$ calculated coincides with $\exp(-t/\tau)$ that is theoretically predicted. The value of $C_v(0)$ is equal to $\frac{1}{3} V_F^2$, corresponding to the average square velocity component $\langle V^2 \rangle$. This accounts for the choice of the normalization value. For $\gamma=0$ the time τ is essentially the correlation time.

Let us consider the curves $C_v(t)$ when $\gamma \neq 0$. With γ increased, i.e., with the film thickness diminished, the decay time decreases. The diffuse electron scattering at the boundaries results in decreasing the effective mean free path and accordingly the characteristic correlation time. The functions $C_v(t)$, however, are not approximated by an exponential, the greater γ , the larger is the deviation from the exponential function.

The autocorrelation functions $C_v(t)$ for $\gamma=10$ and for various specular parameter p , are presented in Fig. 2(a). The specular reflections change the sign of the transverse velocity component but do not randomize the velocity. The longitudinal velocity component, used to estimate $C_v(t)$, keeps the value after reflection in this case. Hence

the correlation time and correspondingly the decay time of the autocorrelation function are only determined by diffuse reflections at the boundaries and by collisions in the bulk. When the diffuse scattering is vanished ($p = 1$), the calculated values of $C_v(t)$ exactly coincide with those calculated for $\gamma = 0$, i.e., for unbounded (infinite) sample. This is in accord with the Fuchs theory, that gives the resistivity of thin film with fully specular surfaces to be equal to the resistivity of unbounded sample, if the Fermi surface of the material is spherical. The decay time decreases with decreasing the surface specularity. At the fully diffuse surface scattering ($p = 0$) the autocorrelation function takes on the limit curve which is determined by both the bulk scattering and the transfer transport of the electron.

In Figs. 1(b) and 2(b) the noise spectral density $S_v(\omega)$, corresponding to the autocorrelation function $C_v(t)$ in Figs. 1(a) and 2(a), are shown.

For $\gamma = 0$, when $C_v(t)$ is defined by

$$C_v(t) = \frac{1}{3} V_F^2 e^{-t/\tau}, \quad (12)$$

the corresponding $S_v(\omega)$ is a Lorentzian:

$$S_v(\omega) = \frac{4}{3} V_F^2 \tau \frac{1}{1 + \omega^2 \tau^2}. \quad (13)$$

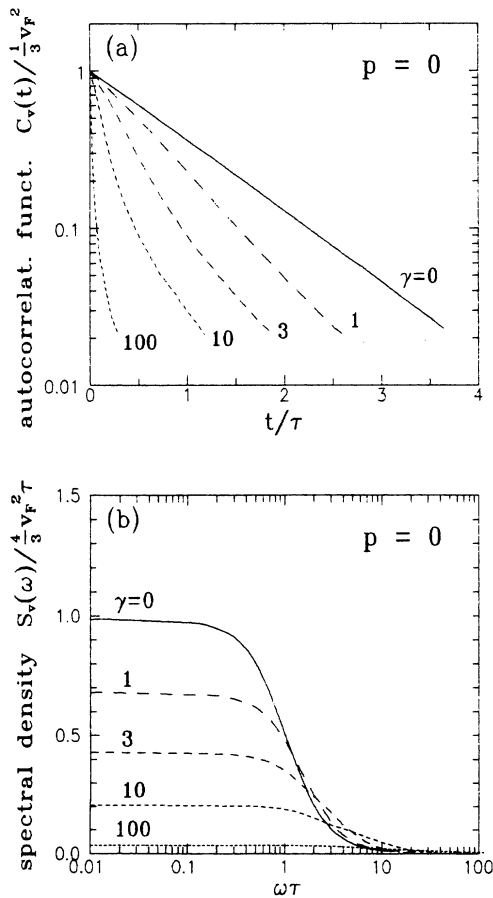


FIG. 1. Autocorrelation function (a) and spectral density of velocity fluctuations (b) calculated within the Fuchs model for fully diffuse boundary scattering and for different γ .

The function obtained coincides nicely with this Lorentzian.

The value of $S_v(\omega)$ in the limit $\omega \rightarrow 0$ is related to the diffusion coefficient of the particle in the unbounded sample by²³

$$S_v(\omega)|_{\omega \rightarrow 0} = 4D. \quad (14)$$

In our case $D = \frac{1}{3} V_F^2 \tau = \frac{1}{3} V_F \lambda$, that corresponds to the expression for classical diffusion coefficient in kinetic theory of gases.

For the case of diffuse scattering the magnitude of $S_v(\omega)$ can be seen to decrease at low frequencies and to increase at high ones when the film thickness diminishes [Fig. 1(b)]. The similar behavior occurs with decreasing p for fixed γ [Fig. 2(b)]. The total area under the curve $S_v(\omega)$, i.e., the integral noise, corresponds to the value of $C_v(0)$ and coincides with the dispersion of random value V :

$$\frac{1}{2\pi} \int_0^\infty S_v(\omega) d\omega = C_v(0) = \langle V^2 \rangle. \quad (15)$$

This quantity remains constant with varying γ and p . Thus in the case under view, the presence of diffusely scattering surface results in the noise redistribution toward higher frequencies with the integral over spectrum

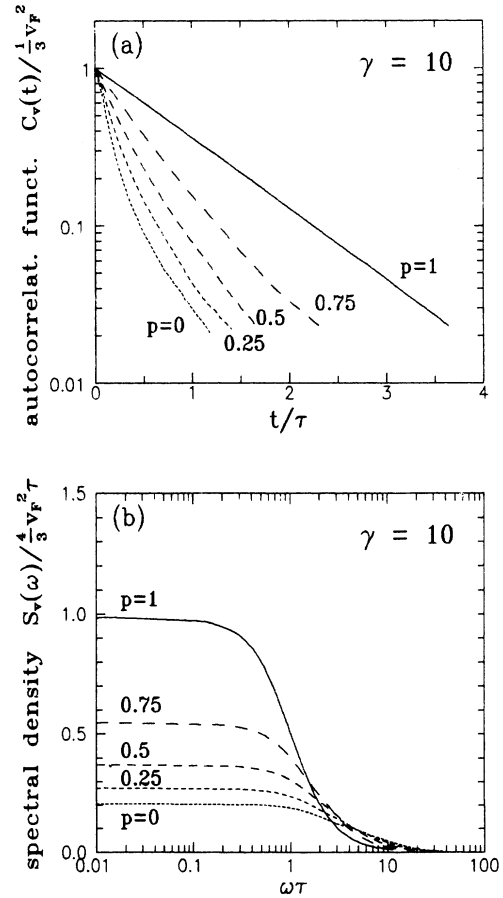


FIG. 2. Autocorrelation function (a) and spectral density of velocity fluctuations (b) calculated within the Fuchs model for $\gamma = 10$ and for different specular parameter p .

being constant. The main consequence of this redistribution is the low-frequency noise being suppressed.

It is known that the fluctuations of the system under thermal equilibrium have to be expressed through the linear response of the system to an external perturbation. This follows from the fluctuation-dissipation theorem.²⁴ The electron system considered in our work corresponds to the equilibrium one, because of the electric field being weak and the deviation of the electron distribution function from its equilibrium being small. Hence the value of spectral density of the drift velocity fluctuations at $\omega \rightarrow 0$ would be expected to be proportional to the drift velocity itself. In order to compare these quantities we use the results for the resistivity of the thin metal film obtained within the Fuchs model and given in Ref. 3. In Fig. 3 the electron drift velocity V_d (inversely proportional to the resistivity) and the low-frequency noise spectral density $S_v(0)$, normalized to the bulk values, are presented as the functions of the film thickness (in units of λ). The curves are shown for two different values of specular parameter: $p=0$ and $p=0.75$. A good coincidence directly indicates the high accuracy of the Monte Carlo algorithm and the validity of the fluctuation-dissipation theorem at low frequencies. These results allow us to use the analytic formulas, obtained for the thin-film resistivity to estimate $S_v(0)$ in some limiting cases. Using expressions for the resistivity given in Ref. 3, one can write for $\gamma \gg 1, p \ll 1$,

$$S_v(0) = V_F^2 \tau \frac{\ln \gamma}{\gamma} (1 + 2p); \quad (16)$$

for $\gamma \ll 1$,

$$S_v(0) = \frac{4}{3} V_F^2 \tau [1 - \frac{3}{8} \gamma (1-p)]. \quad (17)$$

We may take into account that the average electron collision frequency is determined by both the average collision frequency in the bulk and that at the boundaries. From this relation and using (11) one can obtain the formula for the average effective collision time τ^* :

$$\tau^* = \frac{\tau}{1 + (1-p)\gamma/2}, \quad (18)$$

that is virtually the correlation time (characteristic time of velocity chaotization). Although the conductivity calculated by using τ^* is very close to that obtained from the precise formula of Fuchs²⁵ [the same is valid for $S_v(0)$ due to fluctuation-dissipation theorem], the autocorrelation function, however, is not approximated by $\exp(-t/\tau^*)$ and the noise spectral density as a function of frequency is not precisely approximated by an equation like (13). To obtain the noise characteristics one has to do numerical calculations.

The contribution of the transfer transport into $S_v(\omega)$ becomes more important comparable with the bulk scattering, the smaller the thickness d . For $\gamma \gg 1$ the value of $S_v(0)$ is basically determined by transfer transport and the decay time of $C_v(t)$ is approximately equal to $2d/V_F$.

Consider finally the results obtained for the *Soffer boundary condition*. The autocorrelation function $C_v(t)$

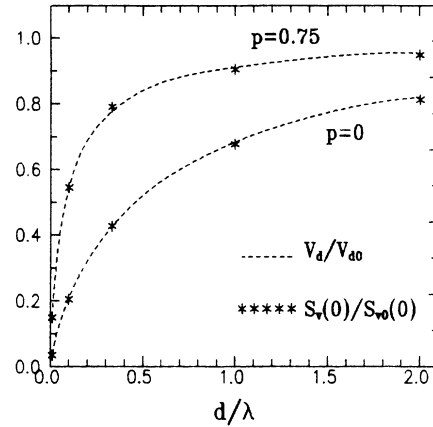


FIG. 3. Low-frequency noise spectral density $S_v(0)$ calculated in the present work (stars) and electron drift velocity V_d taken from Ref. 3 (dashed lines) as the functions of the film thickness d (in units of λ).

and the corresponding noise spectral density $S_v(\omega)$ for $\gamma = 10$ and for various surface roughness R are presented in Fig. 4. The surface is seen to be fully specular ($p \approx 1$) when $R \lesssim 0.01$, that corresponds to a large electron wavelength in comparison with the surface rms height deviation ($\lambda_0 \gtrsim 100h$). In this case $C_v(t)$ (curve 1) coincides with that for the unbounded sample. On the contrary the surface scattering is fully diffuse when $R \geq 2$, that is, when $\lambda_0 \leq 0.5h$. In this case $p \approx 0$ and curve 7 in Fig. 4(a) coincides with that calculated for the Fuchs boundary condition [Fig. 2(a)].

We may also compare the results of both models for an intermediate case of surface roughness if the specular parameter of the Soffer model (1), integrated over the angles of incidence, is equal to that of the Fuchs model. In such a case the total number of specularly reflected electrons are the same for both models, but their angular distributions are different. The Fuchs curves (dashed lines) for $p=0.5$ (α) and $p=0.75$ (β) correspond to the Soffer ones for $R=0.06$ and $R=0.1$, respectively, in Fig. 4. The functions $C_v(t)$ obtained for the Fuchs boundary condition can be seen to decrease more rapidly and the noise redistribution is therefore greater.

The results for an intermediate case of surface roughness ($R=0.2$) and for various film thickness are shown in Fig. 5. The Fuchs curves (dashed lines) for the corresponding $p=0.16$ are also presented. The similar behavior we can see, as before. The greater γ the faster decrease of $C_v(t)$ for the Fuchs model in comparison with that for the Soffer one and the greater the noise redistribution.

The Soffer curves $C_v(t)$ at $t > \tau$ can be seen to become parallel. That means for any γ the autocorrelation functions at large times are exponents with the same decay time being equal to τ . It can be explained by the following way. The main contribution to the autocorrelation function at large times arises from electrons which move at grazing incidence, time and again specularly reflected, so that their free path remains of the order of the bulk free path. In such a case the low-frequency noise suppression is therefore less.

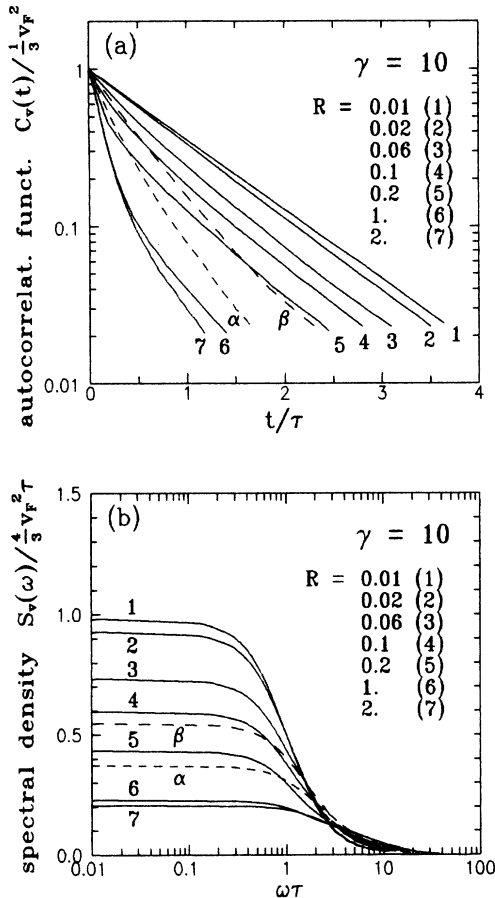


FIG. 4. Autocorrelation function (a) and spectral density of velocity fluctuations (b) calculated within the Soffer model (solid lines) for $\gamma=10$ and for different surface roughness R . Dashed lines are the curves obtained within the Fuchs model for $p_r=0.5$ (α) and $p_r=0.75$ (β).

V. CONCLUSIONS

The current fluctuations in thin metal films have been investigated under size effect. The existing Monte Carlo approach has been extended into the Knudsen regime of electron transport, when the electron scattering at the boundaries prevails over that in the bulk. Under this condition the main characteristics of the noise: autocorrelation function and spectral density of fluctuations have been calculated for various film thickness and surface roughness. The Fuchs and the Soffer models for electron surface scattering were considered. The autocorrelation function for a thin film ($d < \lambda$) was shown to be not exponential in distinction of that for an unbounded sample and the corresponding noise spectral density is not Lorentzian. With diminishing the thickness d and with decreasing the surface specularity, the noise redistribution toward higher frequencies is demonstrated to occur. Suppression of low-frequency noise under the size-effect conditions may be essential and reach up, for

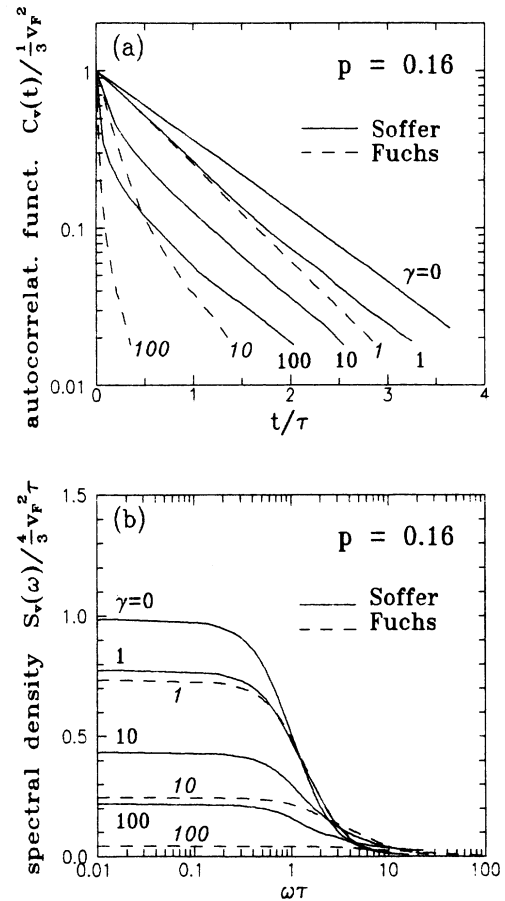


FIG. 5. Autocorrelation function (a) and spectral density of velocity fluctuations (b) calculated within the Soffer model (solid lines) for an intermediate case of surface roughness ($R=0.2$) and for various film thickness. Dashed lines are the curves obtained within the Fuchs model for $p_r=0.16$.

example, several times at $d \sim \lambda$ and tens of times at $d \sim 0.01\lambda$ under the diffuse surface scattering. The fluctuation-dissipation theorem was shown to be satisfied at low frequencies. It is interesting to note that using the above-obtained results and the fluctuation-dissipation theorem for arbitrary frequencies one can easily calculate the frequency dependence of the film conductivity $\sigma(\omega)$ [or more precisely, $\text{Re}\sigma(\omega)$]. All mentioned size dependences and other features are also characteristics for $\sigma(\omega)$. Particularly from these results one can obtain the increase of $\text{Re}\sigma(\omega)$ in the high-frequency region at $d < \lambda$.

The results of the present work can be applied to the study of noise phenomena not only in metal films but in semiconductor ones and other microdevices where the classical size effect is essential.

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