On permittivity of a stacking nano-faulty film

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Theoretical framework is introduced to explain high effective permittivity of a stacking nano-faulty semiconductor film. Effective permittivity dependence on the temperature is shown to be a step-like function with levels determined by the sum parts of constituent layers with relatively high resistivity in film thickness within given temperature region because they are short-circuited by the relatively low resistive layers. These levels at sufficiently low and sufficiently high temperatures coincide with material's true permittivity while at intermediate temperatures may significantly exceed its value. In chemically pure or homogeneously doped coarse-crystalline semiconducting films, the layers distinguished by resistivity can be formed due to piezoresistance effect induced by the local elastic stresses which are related with stacking nano-faults existing in film's plane.
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1. Introduction

In general, reducing of the sizes both of integrated circuits logic devices and memory elements yields their improved performance. However, such advanced "scaling" simultaneously reduces thickness of the insulator films used for gate or capacitor dielectrics what can be compensated only by the substantially increasing in permittivity [1]. Many materials, like the simple and nitrided metallic oxides and silicates, were under the consideration as potential replacements for ultrathin (nanometric) dielectric films in gate and capacitor stack-structures. In recent years, perovskite-type and some related complex materials have attracted much attention due to their extremely high permittivity at low frequencies unchanged over the quite wide temperature ranges.

Namely, high permittivity had been found in oxides of the type $ACu_3Ti_4O_{12}$ (and in isostructural compounds $ACu_3Ti_3FeO_{12}$) [2]. The most exceptional behavior was exhibited by $CaCu_3Ti_4O_{12}$, which shows a permittivity at frequency of ~ 1 kHz of about ~ 12000 that is nearly constant from room temperature. The cubic structure of these materials is related to that of perovskite ($CaTiO_3$), but TiO_6 octahedra are tilted to produce a square planar environment for Cu^{2+} ion. According to the neutron powder diffraction studies, the $CaCu_3Ti_4O_{12}$ structure down to ~ 35 K remains cubic and centric. As for the compositions of the type $A_{2/3}Cu_3Ti_4O_{12}$ (where A is the trivalent rare earth or Bi), most of them show permittivity above ~ 1000. Cubic $CaCu_3Ti_4O_{12}$ possesses a low-frequency permittivity ~ 10^4, which is only weakly varying in the temperature range 100–400 K, but below ~ 100 K, there is an abrupt ~ 100-fold reduction in the value [3]. Thermodynamic and X-ray data argue against an explanation in terms of ferroelectricity, i.e. collective ordering of local dipole moments. Both the low-frequency dielectric response as well as Raman scattering data suggest the existence of highly polarizable relaxional modes with a characteristic gap. Optical conductivity measurements on the perovskite-related oxide $CaCu_3Ti_4O_{12}$ provide a hint of the physics underlying the observed giant dielectric effect in this material [4]. A low-frequency vibration displays anomalous behavior, implying that there is a redistribution of charge within the unit cell at low temperature. At infrared (THz) frequencies, the value for the permittivity was found to be ~ 80 at room temperature, which is far smaller than the value of ~ 10^5 obtained at lower radio (kHz) frequencies. This discrepancy implies the presence of a strong absorption at very low frequencies due to dipole relaxation. At room temperature, the characteristic relaxation times are fast (≤ 500 ns) but increase dramatically at low temperature, suggesting that the large change in permittivity may be due to a relaxor-like dynamical slowing down of dipolar fluctuations in nano-size domains. In wide region above 100–150 K, thin $CaCu_3Ti_4O_{12}$ epitaxial films have a temperature-independent permittivity of the order of ~ 1500 [5], making this material a good candidate for applications. Note that its frequency dependence at lower temperatures indicates an activated relaxation process. Impedance spectroscopy on cubic perovskite-type ceramics $CaCu_3Ti_4O_{12}$ has demonstrated [6] that they are electrically heterogeneous and consist of semiconducting grains with insulating grain boundaries. The giant permittivity values in excess of ~ 10^4 up to kHz-frequencies have been therefore attributed to an internal barrier layer capacitance instead of an intrinsic property associated with the crystal structure. It is a room temperature value, which drops to about ~ 100 below ~ 100 K. The large temperature-independent, low-frequency permittivity observed in $CaCu_3Ti_4O_{12}$ single crystal is most plausibly interpreted [7] as arising from spatial inhomogeneity of its local dielectric response. Probable sources are various nano-domain boundaries endemic in such materials: twin, Ca-ordering, and antiphase boundaries. In general, the material in, and neighboring, such boundaries can be insulating or conducting. Constructed all possible internal morphologies yield dielectric behavior consistent with observations. The further experiments are needed to distinguish between them. Using transmission electron microscopy neither in $CaCu_3Ti_4O_{12}$ single crystals, nor in polycrystalline samples, included sintered bulk and thin films, it has been observed twin domains. Nevertheless, it was found [8] very high density of dislocations, as well as regions with cation disorder, lattice displacements introduced by the planar defects, and grain boundaries with oxygen deficiency, in comparison with grain interior. Obviously, the defect-related structural disorders and inhomogeneity, serving as an internal barrier layer capacitance

in a semiconducting matrix (and supporting morphological model with percolating-conducting regions and blocking regions), might explain the very large dielectric response of the material.

Substituting Cd for Ca reduces the room temperature value of permittivity by over an order of magnitude [9]. The origin of the large permittivity may be due to an internal barrier layer capacitance effect: infrared measurements on the Ca and Cd compounds showed that low-frequency modes increase dramatically in strength at low temperatures, suggesting a change in the effective charges and increasing electronic localization that may lead to a breakdown of the effect.

Copper phthalocyanine based composites also display high permittivity, of order of several hundreds. In an attempt to determine whether they have a high permittivity intrinsically, and if so, in order to identify the circumstances under which such high permittivity could result, a systematic ab initio study was undertaken in [10]. The tendency of Cu-phthalocyanine and closely related H_2-phthalocyanine monomers, and polymeric sheets as well to stack was critically assessed, and the concomitant changes in the electronic and optical properties as a function of the stacking distance were determined. Obtained results indicate that both considered monomer systems exhibit an insulator to metal transition as the stacking distance approaches the equilibrium spacing. Consistent with this behavior, the permittivity reach large values as the stacking distance approaches equilibrium spacing, while it is small for larger distances.

Dielectric relaxations of charge-ordered $Ln_{1.5}Sr_{0.5}NiO_4$ (Ln = La and Nd) ceramics were investigated over a broad temperature range [11] (see also [12]). The high permittivity (over ~ 70000) with a low dielectric loss of ~ 0.1 was determined at high frequencies (up to 5 MHz) over a broad temperature range. There are found two dielectric relaxations in the vicinity of charge ordering temperatures. The thermal activated small polaronic hopping between two charge ordering temperatures should contribute to the giant dielectric response in the present ceramics. Compared to other giant permittivity materials, these materials have the notable advantage for high frequency applications.

A giant low-frequency in-plane permittivity, ~ 10^6, for epitaxial thin films $Ca_{1-x}La_xMnO_3$ ($x < 0.03$) also has been observed [13] over a broad temperature range. This phenomenon was attributed to an internal barrier-layer capacitor structure, with Schottky contacts semiconducting grains. The measured increasing in permittivity with electron- (in this case, La-) doping exceed that of conventional two-phase materials (based on $(Ba,Sr)TiO_3$, $CaCu_3Ti_4O_{12}$ or (Li,Ti)-doped NiO).

Thickness dependence of the permittivity was analyzed [14] for the case of epitaxial $Pb(Zr,Ti)O_3$ thin ferroelectric films and it was shown that the frequency dependence of the measured capacitance is best simulated by an equivalent circuit incorporating the trap-containing capacitance of a Schottky contact (the presence of traps was evidenced by a photovoltaic effect at subgap wavelengths). The thickness dependence of the permittivity, calculated using the formula of a plane capacitor, appears to be an extrinsic effect due to the interface phenomena in the metal–ferroelectric–metal structure. As for the intrinsic permittivity of the material, it seems to be thickness independent (it was also proven by piezoresponse force microscopy measurements) and of lower value of about 30–40, which is closer to the values estimated from Raman measurements, on the one hand, and from quantum theories of ferroelectricity, on the other hand.

Measurements of the permittivity of multiphased binary and ternary mixed alkali halides, which have found a multitude of applications in optical and electronic devices, have been reported in the temperature range from room temperature to 423 K [15]. It was found that the temperature variation in the binary mixed crystal $(NaCl)_{0.587}(KBr)_{0.413}$ is drastically larger than in any other. This variation was shown to be quantitatively reproducible by means of a simple model, which does not contain any adjustable parameter and solely makes use of the properties of the end members NaCl and KBr.

It has been reported [16] the effects of grain size on high dielectric and related electrical properties of $Li_{0.05}Ti_{0.02}Ni_{0.93}O$ ceramics, which were prepared by a direct thermal decomposition method. The analysis of complex impedance indicated that these ceramics were electrically heterogeneous consisting of conducting grains and insulating grain boundaries. Obtained results revealed that the permittivity increases with the increase in grain size, which can be well described by a relaxation mode; and that the different microstructures resulted in chemical change (e.g., oxygen vacancies) inside the grains, leading to the changes in electrical properties of the ceramics.

Structure and dielectric characteristics of $Ba[(Fe_{0.9}Al_{0.1})_{0.5}Ta_{0.5}]O_3$ solid solution were investigated too [17]. The cubic crystal structure was confirmed in the Al-substituted $Ba[(Fe_{0.9}Al_{0.1})_{0.5}Ta_{0.5}]O_3$ ceramics. The extended giant permittivity step and the significantly reduced room-temperature dielectric loss were obtained in the Al-substituted $Ba[(Fe_{0.9}Al_{0.1})_{0.5}Ta_{0.5}]O_3$ ceramics. These improvements of dielectric characteristics have great scientific significance for potential application of giant dielectric constant materials. Performed *X*-ray analysis has confirmed that the low-temperature dielectric relaxation is originated from the mixed-valent structure of Fe^{2+}/Fe^{3+} and the hopping of the charge carriers between them.

The crystalline structure and dielectric properties of $Sm_{1.5}Sr_{0.5}NiO_4$ ceramics were presented in [18]. These ceramics were refined as orthorhombic phase and it was noted that the orthorhombic strain may change the statue of charge ordering. The temperature-stable giant permittivity (~ 100000) with low dielectric loss of ~ 0.1 was observed at frequency up to 5 MHz over a broad range of temperature (150–500 K) and frequency (100 kHz – 5 MHz). The grain interior should be the dominative factor which contributes the giant dielectric response in these ceramics after the equivalent circuit fitting, and the thermal activated small polaronic hopping related to the charge ordering is that factor. Compared to other giant dielectric materials, the present materials have a great potential in the practical application, especially for the high frequency application.

Thus, there exists the class of film materials which quite often are characterized by the giant values of charge capacity *C*: they noticeably exceed so-called geometric value

$C_0 = \kappa_0 \kappa S / d$ calculated on the basis of film area S and thickness d, and material true intrinsic static permittivity κ. Effective permittivity κ_{eff} can be recalculated from the measured capacity using similar formula $C = \kappa_0 \kappa_{eff} S / d$. Consequently, the ratio of effective permittivity and real one $\kappa_{eff} / \kappa = C / C_0$ is defined by the ratio of measured and geometric capacities. Let note that all above described materials are complex chemical compounds. But, effect of the giant effective permittivity for a long time is known in elemental boron. Then, it may be realized different physical mechanisms of the phenomena.

In the present work, theoretical framework able to explain high effective in-plane permittivity of a film is introduced and the issue is discussed how such effect can arise even in coarse-crystalline and chemically pure material.

Paper is organized as follows. Next Section presents a brief overview of the available studies on effective permittivity of boron. Then, the model of a film inhomogeneous by the resistivity is constructed and values of the internal stresses associated with stacking faults existing in real crystals are estimated. And finally, some concluding remarks concerning such kind high effective permittivity are made.

2. Effective permittivity of boron

To best our knowledge there are no recent studies of other authors devoted to the interesting phenomenon of high effective permittivity in boron samples. As for the early data, they are as following.

The capacity-measurements [19] performed at frequencies of 10^4 and $5 \cdot 10^5$ Hz for elemental boron lead κ_{eff} value between 13 and 14, which seems to be only something overestimated in comparison with κ commonly characteristic for boron in ground-state β-rhobmohedral (β-B) structure. Light refractive index near the absorption edge equaled to 3.3, what corresponds to the high-frequency permittivity of $\kappa_\infty \approx 9.9$. According to the β-B reflectance measurements [20], for waves longer than 25 and shorter than 20 μm $\kappa = 10.0 \pm 0.5$ and $\kappa_\infty = 8.4 \pm 0.4$. This kind of dispersion displays non-equivalency of the boron atomic sites in extraordinary complex unit cell (with 105 regular atoms, what causes dipole moment removing the forbidding putted on the single-phonon optical absorption processes). Capacity of the sample measured in [21] also was agreed with its geometrical value. However, it is impossible to exclude that in this case there were contaminations capable to eliminate inhomogeneity by conductivity inherent to a material. In [22], using capacitor method (in frequency range of $10^6 - 10^7$ Hz) and based on β-B optical reflection spectrum, it was found $\kappa = 10.0 \pm 0.5$ and $\kappa_\infty = 8.0 \pm 0.5$. Note that the difference of $\Delta\kappa = 2.0 \pm 1.0$ again exceeds measurement errors. Elliptical-metrical determination of the macro-crystalline β-B optical constants for wave-lengths from 1.000 up to 0.425 μm specified [23] increase in refractive index approximately from 2.7 up to 3.2. It corresponds an interval of $\kappa_\infty = 7.3 - 10.2$. By same method and also based on measurements of the β-B transparency and reflectance it was revealed [24] that at reduction of the light wave-length from 1.20 to 0.35 μm the reflectance increase from 3.00 to 3.35, what means something different region of $\kappa_\infty = 9.0 - 1.2$. Applying contactless techniques of perturbation by the microwave resonator for β-B spherical sample κ has been measured at $9.5 \cdot 10^9$ Hz [25]. Specified frequency is noticeably low in comparison with the value corresponding to the edge of transition from κ to κ_∞ (i.e. to wave-length of 25 μm). Nevertheless, the found value of $\kappa = 8.0 \pm 0.5$ is less than other measured values and is more similar to κ_∞.

In [26], the temperature-dependence of κ_{eff} for β-B macrocrystalline sample was curved based on the total conductivity measurements at the fixed frequency of $4.7 \cdot 10^7$ Hz. At the room temperature it has been found $\kappa_{eff} \approx 15$. With rise in temperature, the step-growth of κ_{eff} was observed. It comes to an end with peak $\kappa_{eff} \approx 30$ at ~ 460 K. Comparison of this curve with results of measurements of internal friction had allowed to connect its features with existence of point defects in combination with dislocations and twins.

Charge capacity together with dielectric losses tangent were measured in temperature interval of 80 – 325 K [27] in polycrystalline boron films, microstructures of which are characterized by the defects in form of dislocations and twinned layers. The peak of losses had been found out, which with increase in frequency (in the range of $5 \cdot 10^2 - 5 \cdot 10^3$ Hz) was displaced toward high-temperatures. Such behavior specifies a relaxation origin of a maximum. As for the capacity, its values to the left of peak are small and practically constant, but to the right of peak – rapidly increase. Further, at the frequency and temperature ranges of $1 - 10^4$ Hz and 80 – 750 K, respectively, these two parameters have been simultaneously measured in zone-melted and film samples using the alternating current bridge [28,29]. At frequency of 50 Hz, two peaks have been found out on the dielectric losses curve. In areas of maxima, the sample capacity remained practically constant, but at higher temperatures sharply increased. Both characteristics displaced along a temperature axis with growth in frequency. At frequency of 10^4 Hz, it has been revealed one more relaxation peak of dielectric losses, intensity of which was correlated with concentration of carbon impurities. In higher temperature region, namely at ~ 570 K, there is a non-relaxation peak. At the same point, sample capacity passes through the maximum. The location of these maxima, independent on frequency, coincides with temperature of the well-known effect of the abnormal changes in some properties of β-B. It is necessary to note that the variation of thickness of the zone-melted β-B samples did not render essential influence on dielectric loss peaks. Concerning temperature dependence of the boron films capacity, it is possible to emphasize that they are similar to the curves obtained for massive samples. However, losses in films have somewhat other character. At frequency of $3 \cdot 10^2$ Hz, in boron films it was observed wide relaxation peak, which settles down approximately at half-height of the low-temperature maximum in massive crystals. Existence of such rich spectrum of the dielectric losses maxima should be caused by the complex interactions between point defects, dislocations, and thin twinned layers in polycrystalline β-B.

Step-like temperature-dependence of β-B capacity has been detected [30, 31] for pure single crystals too. Transitions between steps were accompanied by narrow peaks of dielectric losses. Obtained behavior has noted to be unusual for relaxation process: with increase in frequency these peaks were displaced toward low (instead of high) temperatures.

Dielectric losses in β-B alloyed with Cu, Ti, and V up to 5, 10 and 10 wt. %, respectively, were specially investigated in [32]. Measurements were carried out in the interval of 125–275 K. For example, in case of V-doped β-B at frequency of 50 Hz, there are observed high background absorption practically independent on temperature and intensive low-temperature maximum, which at increase in frequency is displaced in the region of higher temperatures. Apparently, V-impurity atoms are connected with vacancies, high concentration of which is characteristic for β-B lattice. On the other hand, relaxation intensity makes impression that the planar defects clusters in B–V system are equivalent to formation of the domain areas.

In [33], the values of β-B charge-capacity at the room temperature depending on frequency of a variable electric field and a constant biasing voltage have been measured for a pure material, macrocrystalline samples, and single crystals. Despite of significant discrepancies by structural perfection and impurity contents, obtained results for all them were practically identical. Capacities measured at low-frequencies and small bias noticeably exceeded corresponding geometrical values and rapidly decreased to this level with increase in frequency (from 10^2 up to 10^5 Hz) and/or constant bias voltage. As at room temperature β-B predominantly realizes a hopping mechanism of conductivity such behavior may be connected with dipole-layers at interfaces between sample and electrodes. In such case, thickness of dipole-layers depends on current carriers' hopping probability, and at increase in frequency have to decrease. But, giant effective value of the β-B capacity seems to be a bulk effect, not a contact one. It has been proved by test of the various electrodes, what had practically no influence on measurement results.

Voltage effect on β-B capacity was suggested earlier [34], in connection with an electric current switching phenomenon. It was established that in this material at relatively low-temperatures (80–250 K) switching is caused by double-injection from contacts, whereas at higher temperatures (250–400 K) current instability possesses a thermal nature. One of experimental arguments also gives β-B capacity–voltage characteristic: near the double-injection threshold, the sample capacity sharply decreases, while during the thermal switching remains approximately constant.

In view of quickened interest in high-κ dielectric (semiconducting) materials, recently we have returned to the problem of effective permittivity in boron films [35–38]. The temperature-dependences of low-frequency dielectric properties of the various series of β-B films, including mostly pure and perfect samples, have been measured and then results have been analyzed within frames of model of the semiconductor inhomogeneous by resistivity [39]. Summarizing all data available for β-B dielectric properties, one can mark out following two main features: (i) polarizing dielectric losses in this material are small and, hence, its true intrinsic permittivity poorly depends on the applied electric field frequency; in any case, it is of order of 10; (ii) as a rule, the effective low-frequency permittivity of the β-B samples are high, noticeably exceeding the values calculated from their geometry. The conclusion has been made that high effective permittivity of real β-B crystalline films are caused by the presence of planar defects leading to their nano-scale inhomogeneity. It should be emphasized a correlation between experimentally obtained abrupt change in effective permittivity around room temperature and theoretically predicted [40, 41] intrinsic structural phase transition in β-B, which takes place in same temperature region and changes pattern of the partially occupied (vacant) atomic sites.

Now leaving behind the problems of applicability (like the barrier height, carrier mobility, thermodynamic stability, morphology, electrode and technological processes compatibility, reliability etc) specially of boron films as a dielectric in integrated circuits' active or passive components, we will construct a general theoretical framework explaining high effective permittivity of a stacking nano-faulty semiconductor film.

3. Theorizing the dielectric properties of a semiconductor inhomogeneous by resistivity

There are known some theoretical studies devoted to the explanation high permittivity values obtained in various film-materials.

Based on calculations of the shadow image in far field below a thin crystal when a coherent electron source is placed at micrometer distance above the specimen, it was noted [42] that the presence of a planar fault should result in very strong oscillatory contrast (then, using a field-emission electron source in a microscope these predictions were realized in $Bi_2Sr_2CaCu_2O_8$ superconductor containing thin intercalated layers determining lattice displacements at planar faults with accuracy down to ~ 1 pm). In [43], applying a symmetry-based atomic scale theory of lattice distortions it was demonstrated that elastic textures, such as twin and antiphase boundaries, can generate intricate electronic heterogeneities in material with strong electron-lattice coupling, as observed in perovskite manganites and other functional electronic materials. The related problem of computing the effective frequency-dependent conductivity of heterogeneous materials was considered in [44]. To get over the difficulties related with possible broad variations (over many orders of magnitude) of the local conductivities, it was used an efficient method, based on computing the wavelet scale and detail coefficients of the local conductivities. The method identifies the high-conductance paths in a large lattice and reduces it to one that requires far less computation of the effective AC conductivity. In [45], the concept of macroscopic conductivity of heterogeneous media was reexamined and defined with the assessment that the effective properties of randomly inhomogeneous materials are not unique, but scatter within some uncertainty limits; hence, random irregular systems may not have definite percolation thresholds.

The influence of the interface roughness on the charge capacitance between two different dielectric media was investigated [46] assuming roughness fluctuations to be self-affine. It was shown that roughness exponent characterizing short wavelength roughness fluctuations plays the dominant role with respect to the root-mean-square roughness amplitude and the lateral correlation length. Furthermore, it

was shown that any evolution of he interface roughness under conditions leading to time variant local interface slope will have significant influence on charge capacitance properties. An efficient computational method has been proposed within a first-principles framework to calculate capacitances of metal–insulator–metal structures including interfacial effects [47]. In this approach, it was employed metal–insulator models under external electric fields to calculate dielectric responses near the interface region. Macroscopically averaged potentials allow for evaluating the capacitance and local permittivity values of the corresponding capacitor. As the achievement of sufficient capacitance–voltage linearity in metal–insulator capacitors with high permittivity dielectrics is still a challenge, based on fundamental physical mechanisms, such as electrostriction, Coulomb interaction between electrodes, and nonlinear optical effects, a microscopic model, which describes the nonlinearities in capacitance–voltage characteristics of high-κ capacitors, has been presented in [48]. The extended model, which includes stacked high-κ dielectrics and interfacial layers, is able to predict the quadratic voltage–capacitance coefficients as functions of the permittivity.

There are constructed some models of the inhomogeneous dielectrics explaining their high permittivity values. In [49], a capacitor device was modeled consisting of a close-packed arrangement of spheres as the dielectric layer. The top electrode was deposited directly on the upper half of the top layer of spheres and bottom electrode was a flat conductor. Expressions are derived for the capacitance for multiple layers of spheres. The model predicts a decrease in capacitance as the number of sphere layers increases. A semiclassical double-well model of dielectric relaxation current in glasses has been extended [50] to nonzero temperature, complex bias histories, and strong electric fields. For a sinusoidal electric field, thermal excitation gives a contribution to the permittivity that varies having a real part that varies logarithmically with frequency and an imaginary part that varies as the inverse tangent of frequency. These analyses lead to a number of testable predictions, and should be useful for understanding the phenomenon of dielectric relaxation and its impact on electronic devices. An analytical model to interpret nano-scale capacitance microscopy measurements on thin dielectric films has been presented [51]. The model displays a logarithmic dependence on the tip-sample distance and on the film thickness-permittivity ratio and shows a good agreement with finite-element numerical simulations. Another analytical model based on an equivalent capacitance circuit for expressing a static effective permittivity of a composite dielectric with complex-shaped inclusions was suggested in [52]. The geometry of the capacitor containing a composite dielectric was discretized into partial parallel-plate capacitor elements, and the effective permittivity of the composite was obtained from the equivalent capacitance of the structure. First, an individual cell diphasic dielectric (a high-permittivity spherical inclusion enclosed in a lower permittivity parallelepiped) was considered. The capacitance of this cell was modeled as a function of an inclusion radius/volume fraction. The proposed approach is extended over a periodic three-dimensional structure comprised of multiple individual cells. The results of modeling were compared with results obtained using different effective medium theories, series and parallel mixing rules. The equivalent capacitance model may be applied to composites containing inclusions of any geometry and size. Although the method is at static electric field, it can be generalized for prediction of frequency-dependent effective permittivity.

But, quoted models do not cover case, when film is inhomogeneous by the resistivity.

Let us, consider a semiconductor film as a dielectric with variable resistivity. According to the general theory of inhomogeneous semiconductors (see, for example, [53]), film's electric capacity C and dielectric loss tangent tanδ are expressed as following:

$$\frac{C_0}{C} = \sum_{i=1}^{i=n} \frac{p_i \kappa (1+\tan^2\delta)}{\kappa_i (1+\tan^2\delta_i)}, \quad (1)$$

$$\tan\delta = \frac{\sum_{i=1}^{i=n} \frac{p_i \kappa \tan\delta_i}{\kappa_i (1+\tan^2\delta_i)}}{\sum_{i=1}^{i=n} \frac{p_i \kappa}{\kappa_i (1+\tan^2\delta_i)}}. \quad (2)$$

Here κ is the true intrinsic static effective permittivity of the material; n stands for the total number of layers with different resistivity across the bias electric field; κ_i and $\tan\delta_i$ denote i-type layers' permittivity and dielectric loss tangent, respectively; and p_i is the sum part of the i-type layers in film thickness obeying the normalization condition

$$\sum_{i=1}^{i=n} p_i = 1 \cdot \quad (3)$$

Regardless of possible complicated frequency- and temperature-dependences, κ_i values should obey inequalities $\kappa_\infty \le \kappa_i \le \kappa$ where κ_∞ is the true intrinsic high-frequency permittivity of the material.

As for the dielectric loss tangent tanδ in i-type layers, it is expressed by the sum of two terms corresponding to the polarization ($\tan\delta_i'$) and conduction losses, respectively:

$$\tan\delta_i = \tan\delta_i' + 1/\kappa_0\kappa\omega\rho_i \quad (4)$$

Here ρ_i is the conductivity of i-type layers and ω is the cyclic frequency of the applied alternating bias field. On the one hand, the usual relative deviation κ_∞ from κ is slight. On the other hand, in spite of frequency and temperature dependences polarization dielectric losses have to satisfy the inequality $\tan\delta_i' \le (\sqrt{\kappa/\kappa_\infty} - \sqrt{\kappa_\infty/\kappa})/2$. Consequently, polarization losses in any layer should be small and lattice vibration can influence the total dielectric losses in i-type layers (see Eq. 4) only if they are small too. But, in this case, as one can see from Eqs. 1 and 2, the parameters of i-type layers do not affect C and tanδ values. Aiming to consider influence of the inhomogeneous resistivity, we assume the permittivity spatial homogeneity, $\kappa_i \approx \kappa$, and neglect by the polarization losses, $\tan\delta_i' << 1$.

As a result we get the simplified formulas for dielectric parameters:

$$\frac{C_0}{C} \approx \sum_{i=1}^{i=n} \frac{p_i (1+\tan^2\delta)}{1+1/(\kappa_0\kappa\omega\rho_i)^2}, \quad (5)$$

$$\tan\delta \approx \frac{\sum_{i=1}^{i=n} \frac{p_i}{\kappa_0\kappa\omega\rho_i + 1/\kappa_0\kappa\omega\rho_i}}{\sum_{i=1}^{i=n} \frac{p_i}{1+1/(\kappa_0\kappa\omega\rho_i)^2}} \quad (6)$$

By fixing the bias field frequency, on the basis of obtained relations it can be considered the diversity of temperature regions with different resistivity values in layers.

If conduction losses in layers of all types are small, $\kappa_0\kappa\omega\rho_i >> 1$, the total dielectric losses in inhomogeneous semiconductor is small too, $\tan\delta << 1$, while film's capacity approximately equals to its geometric value, $C \approx C_0$.

In contrary, if conduction losses in layers of all types are high, $\kappa_0\kappa\omega\rho_i << 1$, the total dielectric losses should be high as well, $\tan\delta >> 1$, and film's effective capacity should exceed geometric one, $C > C_0$, by the factor of $\sim 1 / p$ where p is the sum part of layers with lowest conductivity.

When conduction losses in part of layers are low, $\kappa_0\kappa\omega\rho_i >> 1$, and in rest of layers are high, $\kappa_0\kappa\omega\rho_i << 1$, the total losses should be low, $\tan\delta << 1$, while capacity again is expressed by the ratio C_0 / p. But, now p denotes the sum part of layers with relatively low (not only with lowest) dielectric losses.

Thus, the temperature dependence of the inhomogeneous semiconductor should be described by a step-like function with levels determined by the sum parts of layers with relatively high resistivity in given temperature region because they are short-circuited by the relatively low-resistive layers. The switch from one level to another takes place in narrow temperature interval where resistivity of a certain k-type of layers meet the condition $\kappa_0\kappa\omega\rho_k \sim 1$. From general Eq. 6 one can see that within this region the dielectric loss tangent may be approximated in following way:

$$\tan\delta \approx \frac{p_k/p}{(1+p_k/p)\kappa_0\kappa\omega\rho_k + 1/\kappa_0\kappa\omega\rho_k}. \quad (7)$$

Here p stands for the sum part of layers with high resistivity, $\kappa_0\kappa\omega\rho_i >> 1$. According to the obtained Eq. 7, the dielectric loss tangent considered as function of resistivity in k-type layers in general has a maximum

$$\tan\delta_{k\ \max} \approx \frac{p_k/p}{2\sqrt{1+p_k/p}} \quad (8)$$

at the temperature corresponding to the k-type layers resistivity value of

$$\rho_{k\ \max} \approx 1/\kappa_0\kappa\omega\sqrt{1+p_k/p}\,. \quad (9)$$

If $p_k >> p$, the value of $\rho_{\max}$ does not meet the condition $\kappa_0\kappa\omega\rho_k \sim 1$. Consequently, peak falls beyond the temperature interval determined by this condition and the maximum does not reveal. But, when $p_k \leq p$ one can find the narrow loss-peak with magnitude of $\tan\delta_k \leq 1/2\sqrt{2}$.

Finally, if there is only one type of layers, i.e. $n = 1$, we dial with homogeneous semiconductor and the film's capacity exactly equates its geometric value, $C = C_0$, while the temperature-curve of the dielectric loss tangent follows to that of the $\rho_1 \equiv \rho$ resistivity, $\tan\delta = 1/\kappa_0\omega\rho$. The situation like this also should be realized even in inhomogeneously doped semiconductors at sufficiently high temperatures when all of layers switch to the intrinsic conductivity.

In general, the dielectric loss in inhomogeneous semiconductor film in dependence on the temperature should follow to that of the specimen conductivity averaged by the certain way. As it is known, semiconductors reveal the monotonous growth in their ohmic conductivity with temperature. However, inside the inhomogeneous semiconductor specimen between two adjacent layers with different ohmic conductivities it can be formed the barrier layer with non-ohmic conductivity which may in unusual way depend on the temperature.

Summarizing above discussion we can conclude that temperature characteristic of the inhomogeneous semiconductor capacity is a step-like function. The step-levels at sufficiently low and sufficiently high temperatures (location of the low-temperature region depends on the bias field frequency) coincide with specimen geometric capacity C_0 while at intermediate temperatures the capacity-levels exceed this value, $C > C_0$. As for same characteristic for loss tangent, in general it reveals growth of the dielectric losses but at least the part of the switches between different capacity-levels should be accompanied by the loss tangent maxima.

4. Planar defects in semiconductor as a source of the inhomogeneous resistivity

There are known number of different physical mechanisms of the inhomogeneous electric resistivity connected with chemical impurities and structural defects in semiconductors like the inhomogeneous doping and impurities segregation, grain boundaries in polycrystalline specimens, as well as formation of complexes of impurity atoms with radiation defects in irradiated material [54] etc, which yield unusual high values of various electro-physical parameters (see, for example, [55]). At the same time, there are strong evidences for resistivity-inhomogeneity effect even in single-crystalline and chemically pure semiconducting films, namely, boron samples. In such cases the layers with different resistivity can be formed only due to piezoresistance effect induced by the local elastic stresses which are related with twinning boundaries and/or stacking faults existing in real single crystals. In adjacent areas of the material, these planar defects create mechanical stresses causing piezoresistance effect sufficient to form inclusions of layers with noticeably increased resistivity. In addition, at borders of such layers with matrix with different (i.e., lower) resistivity can arise barrier layers also with high resistivity. Such kind of inhomogeneity of the real crystalline films by resistivity means an opportunity of electric charge accumulation not only on film's interfaces with electrodes, but also in bulk – at borders between areas with relatively low resistivity and relatively high resistivity. As a result, effective thickness of the equivalent capacitor decreases and measured value of capacity in comparison with geometrical one increases.

The fact is that the real single-crystalline structure can include the twinned nano-layers. Besides, the stacking nano-faults are capable to combine into micro-twins. In both cases the twinning boundary is a symmetry plane for the twin components. Therefore, it seems appropriate the model [56] of simple tilt boundary between the pair of disoriented

single-crystalline blocks constructed from the equidistant edge dislocations: the neighbor dislocations are located at the certain h distance. It should be emphasized that such kind of dislocation assemblies are stable and at the same time do not produce long-range stresses in crystal.

There are useful the Cartesian co-ordinates for which yOz plane coincides with tilt boundary while the component dislocations are directed along the Oz axis. Then, the local dilatation caused by the boundary stresses does not depend on z co-ordinate. However, it is a periodic function of y with periodicity of h and monotonously decreases as the distance $|x|$ from the boundary increases. Particularly, considering isotropic medium we get the relative change in volume in form of

$$\frac{\Delta V(x,y)}{V} = -\frac{1-2\sigma}{1-\sigma}\frac{\sin\theta/2\ \sin 2\pi y/h}{\cosh 2\pi x/h - \cos 2\pi y/h}. \quad (10)$$

Here σ is the material Poisson coefficient and θ is the structure turning angle at the boundary. It should be noted that according to this expression the dilatation is divergence at the isolated points $y = nh$ ($n = 0,\pm1,\pm2,..$) located exactly on the $x = 0$ boundary. This effect is related with inapplicability of the theory of elasticity at the distances comparable with inter-atomic like the dislocation core radius. But, inside the overwhelming part of stressed region the first term $\cosh 2\pi x/h$ of the denominator in Eq. 10 significantly exceeds the second one $\cos 2\pi x/h$, and neglecting by latter we can obtain the approximated expression with quite physical behavior at the boundary. We extrapolate it for ultra-short $|x|$ distances too. Now we can average out absolute value of the dilatation by y within the range of periodicity $0 \le y \le h$:

$$\left|\frac{\Delta V(x)}{V}\right| = \frac{2}{\pi}\frac{1-2\sigma}{1-\sigma}\frac{\sin\theta/2}{\cosh 2\pi x/h}. \quad (11)$$

One can see that function expressed by Eq. 11 has a wide maximum at the boundary and rapidly (nearly exponentially) decreases at large distances from the boundary. Consequently, in good approximation it can be substituted by the step-like function which equals zero at large distances and non-zero constant $\delta \equiv \Delta V(0)/V$ within the certain finite region symmetric against boundary. The width of the dilatation constancy region

$$x_0 = h/2 \quad (12)$$

is determined by equating the areas under the graphs of exact and approximate functions.

Introducing of the constant dilatation allows find the internal pressure value $p = K\delta$ within the stressed regions. Here K denotes the compression bulk modulus which is determined via the Young's modulus E as $K = E / 3(1-2\sigma)$. Thus, the pressure inside the layer with width of $h/2$ and centered at the defect's plane can be calculated as follows

$$p = \frac{2\sin\theta/2}{3\pi}\frac{E}{1-\sigma}. \quad (13)$$

Eqs. 13 and 14 should be used for estimates of the piezoresistance effect in regions adjacent to the twinning boundaries and stacking planes in semiconductor crystals.

5. Concluding remarks

Summarizing obtained results it should be stated that effective permittivity of the semiconductors inhomogeneous by resistivity spatial distribution is expected to be a step-like function of temperature with levels determined by the sum parts of layers with relatively high resistivity. At the intermediate temperatures these levels may lay significantly higher than permittivity value calculated from the specimen geometric form and sizes neglecting by its inhomogeneity. The part of switches between different permittivity-levels may be accompanied by the dielectric loss tangent maxima.

In chemically pure or homogeneously doped single-crystalline semiconducting films the layers with different resistivity should be formed due to piezoresistance effect induced by the local elastic stresses connected with planar defects – nano-faults and/or micro-twins.

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Stószolt, nano-hibahelyes film permittivitásáról
Elméleti megfontolások alapján értelmezzük egy stószolt, nano-hibahelyes félvezető film nagy tényleges permittivitását. Kimutatjuk, hogy az effektív permittivitás a hőmérséklet függvényében lépcsős függvény szerint változik. A függvény szintjeit a filmalkotó rétegek összegrészei határozzák meg; e rétegek az adott hőmérséklet-tartományban viszonylag nagy ellenállásúak, mivel a viszonylag kis ellenállású köztirétegek rövidre zárják azokat. A szintek eléggé alacsonyak, és ha a hőmérséklet elég magas, a kapott permittivitások jól egyeznek az anyag tényleges permittivitásával, míg közbenső hőmérsékleteken jelentősen meghaladhatják azt. Kémiailag tiszta, vagy homogénen adalékolt durvakristályos félvezető filmekben a különböző ellenállású rétegek piezoellenállás eredményeként alakulhatnak ki, helyi elasztikus feszültségek hatására; e feszültségek a film síkjában megjelenő nano-hibahelyekkel függnek össze.
Kulcsszavak: félvezető film, stószolt nano-hiba, effektív permittivitás

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