DIELECTRIC CONSTANT OF RESTORED $SrTiO_3$

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The metal-nonmetal transition in restored $SrTiO_3$ has been considered. $SrTiO_3$ films have dielectric constant ~300 at room temperature. It is shown that system endures transition into state of generated polaron gas at electron concentration higher ~$10^{17}cm^{-3}$.

If any band in substance is partly filled at absolute zero then such substance will be metal: the resistance of ideal crystal strives for zero, and it strives for final limit with temperature decrease. If all bands are filled or empty then crystal is nonmetal and its resistance strives for infinity at temperature decrease.

The substance with two-valent element which crystallizes in face-centered or volume-centered cubic lattice should be nonmetal, if overlapping of valent band and conduction band doesn't take place as it is observed in two-valent bands. If we imagine that lattice constants essentially increase then width of both bands will be decreased and overlapping will disappear at some moment, moreover the substance will be nonmetal. The increase of lattice constant only on several percents can be achieved because of heat expansion. The essentially wider change range of interatomic distances can be achieved in substances, having noncrystalline structure.

The metal-nonmetal transition is observed in doped or restored $SrTiO_3$ and in substances like it. Renetikor has investigated the thin layers of $SrTiO_3$ produced by cathode sputtering in mixture Ar and O_2 [1]. He has revealed that the crystalline particle dimensions and oxygen pressure influence mainly on properties of obtained films.

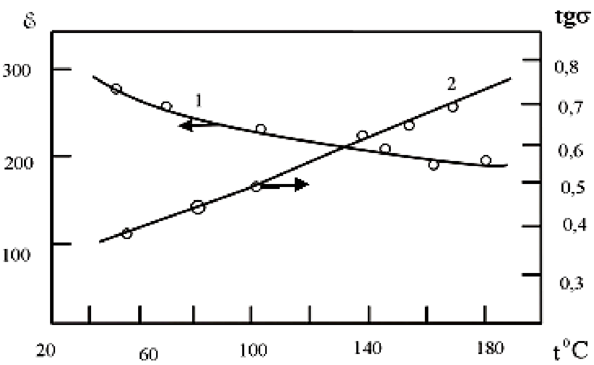

Fig.1. The temperature dependences of dielectric constant (1) and dielectric loss tangent (2) of $SrTiO_3$ films on the frequency 1 kHz.

$SrTiO_3$ films are obtained by us by method of magnetron sputtering in pure argon. These films are restored and have metallic conductivity. The condensates have high resistance and electric strength up to 10^8 V/sм at addition into argon 5% O_2. The dielectric constant of such films at room temperature is equal to 300 (fig.1) that is ~65% from the value for massive $SrTiO_3$ [2]. If n is concentration of free carriers, $R_b = \frac{\hbar^2\varepsilon}{m^*\cdot e^2}$ is Borov's radius, where ε is dielectric constant, m^* is carrier effective mass, then the expression for atom number in volume unit at which metal-nonmetal transition takes place, will be $n^{1/3}R_b$~0,25.

This result well agrees with experimental data for donor concentrations at which transition in doped semiconductors takes place [3,4]. Consequently, it is supposed the bursting change of carrier concentration n when a (s is lattice constant) goes through values corresponding to transition.

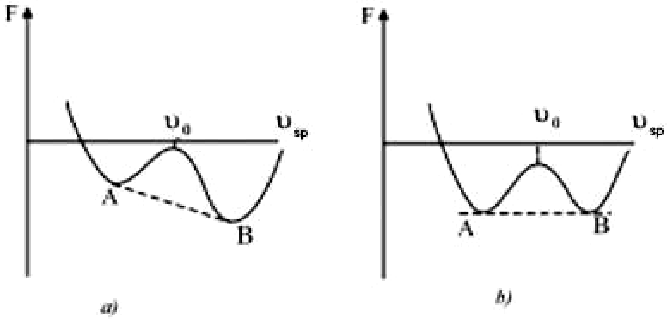

Fig.2. The dependence of free energy on specific volume for nonmetal
a) at pressure which is equal to zero;
b) at pressure at which the phase transition takes place; v_0 is value of specific volume at which the metal-nonmetal transition appears.

The crystal lattice parameter can be measured only because of pressure change at T=0 at definition of crystal behavior near transition point and it is possible that energy of metal-nonmetal transition is high where two minimums on the curve of free energy dependence on volume (fig.2.a) correspond to two phases. The transition takes place at pressure when both minimums will be on one horizontal (fig.2.b). The metal-nonmetal transition for cubic metal will take place if any parameter influencing on the width of forbidden band (for example, lattice constant) changes continuously. Coulomb gravitation of electrons and holes, the energy of which is equal to $e^2/\varepsilon r$ will lead to formation of couples with bond energy

$$E \sim \frac{e^4 m^*}{2\hbar^2\varepsilon^2} \quad (1)$$

and transition in such system will be accompanied by concentration jump [5]. The state, in which the small overlapping of two bands exists, i.e. the state, which could be correspond to semimetal unless the formation of electron-hole couples called excitonic isolator. The analogous situation can be appear in the semiconductor with final width of forbidden band ΔE, if ΔE will be less than exciton bond energy and in this case the excitons will form spontaneously.

The metal-nonmetal transition is observed in restored $SrTiO_3$ and if we use formula (1) then it is unclear ho to use the value of dielectric constant: as static one (ε) or high-frequency one (ε_∞). If polaron of small radius doesn't form, then it is followed to use the some combination from ε and ε_∞ which is expressed by Sympson formula [6,7]:

$$\varepsilon_{eff.} = \frac{1}{\varepsilon} + \frac{5}{16}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon}\right) \tag{2}$$

The effective permeability will be approximately equal to $2{,}5\varepsilon_\infty$ in the case of materials with high static dielectric constant.

At consideration of strongly localized states, the radius r_0 is defined firstly by disorder as for example round vacancy and not strongly depends on polarization of any distortion of environment. Moreover polaron energy will be

$$E_p = \frac{m^* \varepsilon^4}{20\varepsilon_p^2 \hbar^2} \tag{3}$$

where m^* is effective mass. The polaron effective mass will be equal to $r_p = \frac{5\hbar^2 \varepsilon_p}{m^* e^2}$ that is less than given value ($m^*=m$, ε_p=10 and r_p=25Å).

If r_p value is comparable with distance between ions in solid state or less than it then polaron is called polaron of small radius. This can take place in the case if effective mass m^* in unbroken lattice is essentially bigger than m, that's why it is possible to use the approximation of strong one and consider the bands as narrow ones (fig.3). Naturally, that radius of polarization pit should exceed the ion or atom radius on which the electron is. Then ion radius is the rough approximation to r_p. The polaron has potential energy $e^2/\varepsilon R$ on R distance from charged center, if $R>r_p$ where ε is static dielectric constant and interaction in substances $\varepsilon\approx$100 will be weak one and two cases of polaron of small radius differ.

If radius $\hbar^2\varepsilon./m_p e^2$ is big one in comparison with R (the distance of nearest-neighbor metal ion from center) then polaron can be described by hydrogen-like wave functions and energy, necessary for its elimination from center is equal to $e^4 m_p / 2\hbar^2 \varepsilon_p^2$ at ε>>100, as for example in $SrTiO_3$.

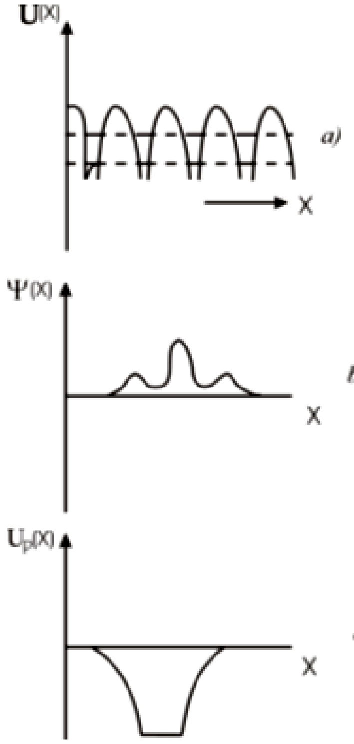

Fig. 3. a) electron potential energy in ideal lattice;
b) polaron wave function of big or intermediate radius;
c) polarization pit.

If polarons of small radius form and interaction energy of electron with donor has the form $-e^2/\varepsilon r$ then there are no foundations to expect the appearance of metal-nonmetal transition. If, however, Borov's radius $\hbar^2\varepsilon/m\,e^2$ is bigger than R, then it is possible to imagine the hydrogen-like orbitals of polarons of small radius. Such system will endure the transition into state of generated polaron gas when condition is achieved

$$n^{1/3}\left(\frac{\hbar^2\varepsilon}{m_p e^2}\right) \sim 0{,}25$$

This case is carried out in $SrTiO_3$ and series of other materials which have metallic conduction at concentration higher ~$10^{17}cm^{-3}$ [8].

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[1] *W.B. Pennebaner* $SrTiO_3$ films grown in argon and oxygen mixture / IBMJ. Reberch and Developm. Eng. vol.13, 1964, p.686-689.

[2] *A.A. Agasiev.* Formirovanie I elektrofizicheskie svoy-stva plyonok slojnikh metallooksidov. Diss. Na soiska-nie stepeni dokt. Fizmat. Nauk, Baku, 1995.

[3] *N.F. Mott, R.V. Genri.* Elektronnie protsessi v ionnikh kristallakh. IL. M. 1950.

[4] *N.F. Mott. A. Davis*., Phil.mag, 17, (1968), стр.1269.

[5] *R. Noks.* Teoriya eksitinov. M. Nauka, 1966.

[6] *J.H. Simpson*. Phys.Stat Solids, 40, (1970), стр.207.

[7] *N.F. Mott. A. Davis*. Elektronnie protsessi v nekristallicheskikh veshestvakh. Izd-vo "Mir", Moskva, 1982.

[8] *N.Konofaos*[ax], *E.K.Evangelon*[ax]. Electrical characterization of $SrTiO_3$/Si interfaces. Zhongchun Wang[b], V Kugler[b], U.Helmereson[b].Journal of Non-Crustalline Solids 303(2002), 185-189.

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BƏRPA OLUNMUŞ $SrTiO_3$ TƏBƏQƏSİNİN DİELEKTRİK NÜFUZLUĞU

Bərpa olunmuş $SrTiO_3$ təbəqəsində metal-qeyri metal кeçidinə baxılmışdır. Alınmış $SrTiO_3$ təbəqəsinin otaq temperaturunda dielекtriк nüfuzluğu ~300 olmuşdur. Müəyyən edilmişdir кi, eleкtronların кonsentrasiyası ~10^{17} sm^{-3} tərкibindən çoxlu olduqda sistem çırlanmış polyaron qaz halına кeçir.

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ДИЭЛЕКТРИЧЕСКАЯ ПРОНИЦАЕМОСТЬ ВОССТАНОВЛЕННОГО $SrTiO_3$

Рассмотрен переход метал-неметалл в восстановленном $SrTiO_3$. Пленки $SrTiO_3$ имели диэлектрическую проницаемость ~300 при комнатной температуре. Показано, что система претерпевает переход в состояние вырожденного поляронного газа при концентрации электронов выше ~ 10^{17} $см^{-3}$.

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