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Anomalous behavior of epitaxial indium nano-contacts on cadmium-zinc-telluride

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In this work, experimental characterization results of indium nano-contacts are presented. The indium nano-contacts are epitaxially grown on a two-dimensional surface of high-resistivity, n-type Cd$_{0.9}$Zn$_{0.1}$Te in ultra-high vacuum. The scaling effect in these contacts is systematic, but not linear. It is shown that the contacts exhibit a profoundly asymmetric behavior. It is argued that the “rectifying” behavior of these contacts is due to tunneling and that the tunneling does not necessarily imply Schottky nature. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4754706]

Cadmium-zinc-telluride (CdZnTe) crystals have been extensively studied since the 80s as a promising material for gamma ray detectors, and as a substrate material for infrared, epitaxial HgCdTe (MCT) detectors. The issue of contacts to Cd$_{1-x}$Zn$_x$Te was found to be critical to the overall performance of the devices. It is widely accepted that indium forms Ohmic contacts on n-type Cd$_{1-x}$Zn$_x$Te when large size contacts are formed on chemically etched surfaces. This understanding is based mainly on the near-linear current-voltage characteristics of macroscopic metal-semiconductor-metal (MSM) devices. Detailed studies of indium contact formation on atomistic level were conducted only recently. It was shown that in ultra high vacuum on two-dimensional Cd$_{0.9}$Zn$_{0.1}$Te surface indium contacts grow epitaxially. However, measuring the characteristics of indium nano scale contacts, having no more than a few atomic layers of thickness on Cd$_{1-x}$Zn$_x$Te is challenging. On one hand the single crystal Cd$_{1-x}$Zn$_x$Te is rather brittle and easily damaged if pressure is applied, and on the other hand indium is soft and thin. Therefore, in full-contact measurements to such contacts the indium layer is practically erased by the contacting tip.

For the current-voltage ($I$-$V$) characterization of the ultra-thin nano-contacts, we have applied successfully the torsion-resonance tunneling atomic force microscopy (TR-TUNA) method, described in more detail in Ref. 6. Using the TR-TUNA mode, we were able to identify very clearly and repeatedly high current clusters that were attributed to nano-contacts. A typical two-dimensional image of TR-TUNA characterization is shown in Fig. 1(a); whereas the superimposed profiles of current-topography along the marked cut are shown in Fig. 1(b). It can be seen that the current contrast is rather high and that there is no clear correlation between the topography and the current readings (excluding cross-talk related artifacts). Following the contact identification, the AFM tip was placed over the contact and the scan area reduced to zero. In this mode, the bias of the tip was scanned relative to the sample in both polarities. The experiment was repeated with numerous contacts of each size in order to examine the uniformity of contact formation process, and to validate the results statistically.

Three aspects of contact $I$-$V$ characteristics were examined: uniformity, general behavior, and scaling. The repeatability of the measurements on the same contact, as well as on different contacts with similar area is excellent, indicating well controlled process and characterization reliability.

All measured contacts exhibit “rectifying-like” behavior. The $I$-$V$ characteristics show nearly perfect exponential dependence in negative polarity (negative bias on the nano-contact) and no measurable current with positive polarity. Measuring all contact currents with a constant tip bias ($\pm 2$ V) and plotting the currents versus area$^6$ yields near linear...
relationship for the larger contacts (above ~30 nm radius). For smaller contacts, the slope seems to increase. In order to study the scaling effects in more details, it is convenient to normalize the full I-V curves to the contact area (obtaining current density, \( J \), versus bias). A typical ensemble of \( J-V \) curves measured for various contacts is shown in Fig. 2. The experimental data points are superimposed with simple exponential fits (represented by lines).

![Graph](image)

**FIG. 2** Experimental \( J-V \) characterization results (experimental I-V results normalized to the contact area). The experimental data points are superimposed with simple exponential fits (represented by lines).

where \( \varepsilon_s \) is the semiconductor’s permittivity, \( N_D \) is the donor concentration (for \( n \)-type), \( q \) is the electron charge, and \( V_t \) is the total potential drop. While the shape of the contacts with \( a < l \) is practically independent of \( N_D \), it is governed by the contact size, \( a \). The general trend of increasing current density with downscaling is fully consistent with tunneling current mechanism and the simulated barrier results. With decreasing contact size, the barrier becomes narrower and the tunneling probability increases, increasing the tunneling current density. Under “forward” bias conditions (positive potential on the nano-contact), the electrons flow from \( \text{Cd}_{1-x}\text{Zn}_x\text{Te} \) into the metal contact with no significant potential barrier; however, the current is limited by the native electron concentration of the semi-insulating \( \text{Cd}_{1-x}\text{Zn}_x\text{Te} \).

Computer calculations set the current, even without velocity saturation effect, below 10 FA, which is below our instrument detection limit. The electric field under a 400 nm \(^2 \) contact at 2 V is calculated to be over 10\(^8 \) V/m, therefore velocity saturation is expected to lower the current significantly. The possibility of increased reverse current in nano-contacts due to non-local tunneling was well demonstrated in the CoSi\(_2\)-Si \textit{Schottky} system (where electron affinity of semiconductor is smaller than the workfunction of the contact). System used in this study (indium–\( n \)-type \( \text{Cd}_0.9\text{Zn}_{0.1}\text{Te} \)) is known to yield “Ohmic-like” contacts in macroscopic dimensions. This seems to be the first experimental evidence of diode-like behavior due to enhanced tunneling induced by downscaling in otherwise “Ohmic-like” systems.

Can these experimental results be quantitatively explained by existing tunneling models? In such case, additional contact parameters could be deduced. Analytical approximations for field emission and tunneling through a \textit{triangular potential barrier} were developed by Fowler and Nordheim. Field emission (FE) and thermionic field emission (TFE) tunneling models for \textit{parabolic potential barrier} shape were developed by Crowell et al. and Padovani et al. The former applies to the MOS structures and the latter to one dimensional \textit{Schottky} contacts (assuming depletion approximation). The latter model can be summarized in the following equations:

\[ J_{TFE} = J_S \times e^{\frac{qV_t}{kT}}. \quad (2) \]

\[ E' = E_00 \left[ \frac{qE_00}{kT} - \tanh \left( \frac{qE_00}{kT} \right) \right]^{-1}, \quad (3) \]

\[ E_{00} = \frac{\hbar}{2} \sqrt{\frac{N_D}{m^*\varepsilon_{\text{CZT}}}}. \quad (4) \]

\[ J_S = \frac{A^* \sqrt{\pi E_00}}{kT} \left( -qV + \Phi_0 \cosh^{-2} \left( \frac{E_00}{kT} \right) \right) \times e^{-\frac{qV}{q_0}}, \quad (5) \]

\[ E_0 = E_{00} \coth \left( \frac{qE_00}{kT} \right). \quad (6) \]

Notations in Eqs. (2)–(6): \( k \)-Boltzmann constant, \( T \)-temperature in Kelvin, \( \varepsilon_{\text{CZT}} \)-permittivity of \( \text{Cd}_{1-x}\text{Zn}_x\text{Te} \), \( \Phi_0 \)-potential barrier, \( A^* \)-Richardson constant, \( q \)-electron charge, \( \hbar \)-reduced Planck constant, \( N_D \)-donor doping concentration (in our case effective doping concentration). Originally, the
parameter $V$ referred to the potential difference between electron quasi-Fermi level ($imref$) in the semiconductor bulk and the energy at which the tunneling occurs (somewhat above the Fermi energy of the metal in the case of TFE). This value reduces to the external reverse bias, $V_r$, in the case of pure FE regime, or for high bias voltages. Later works used the value of $V_r$ instead of $V$ as a reasonable approximation and we will follow this path, because the tunneling in our case occurs at relatively high bias.

However, in the case of nano-contacts the shape of the potential barrier is neither parabolic nor triangular. Furthermore, the approximation of the electrostatic potential profile with the distance, $r$, from the contact as $V \propto a/r$ (where $a$ is the contact dimension) from Ref. 7, is only applicable at distances $r>a$ from the contact. In the most important region (vis-à-vis tunneling), namely just under the contact, the above mentioned approximation is not applicable. Thus it can be concluded that the shape of the barrier in nano-contacts has to be numerically computed as a function of bias; and in addition, there is no known analytical approximation for tunneling current calculations with that barrier shape.

Can we correlate the nano-contact tunneling process to the FE tunneling of large (infinite) Schottky contacts? This could make sense since both, the experimental results of the nano-contacts $J$-$V$, and the FE current dependence of large Schottky contacts are nearly exponential. From the physics viewpoint, the tunneling process mainly depends on the energy band structure that is adjacent to the contact (the nm range where the quantum tunneling takes place), as shown in Fig. 3. The calculations of the energy band diagrams, shown in Fig. 3, were performed using finite element TCAD software. The numerical solution was for 3-dimensional circular shape contacts. More details about computation and physical models used can be found in Ref. 9. While the overall calculated barrier shapes of the nano-contacts are not parabolic, one could fit fairly well the regions of interest of the calculated conduction energy bands to parabolas. This fit defines an effective doping concentration, $N_{D,eff}$, for each nano-contact size. The value of $N_{D,eff}$ is deduced from the textbook Poisson equations for infinite Schottky contact with depletion approximation. Namely, each nano-contact size gets an assigned effective doping concentration (which would yield similar barrier under an infinite contact in the main region of interest). However, this approach does not seem to provide an insight because $N_{D,eff}$ changes with applied bias, and even point by point fit, taking $N_{D,eff}(V_{Bias})$, requires unreasonable barrier modifications. It should be noted that in semi-insulating Cd$_{0.9}$Zn$_{0.1}$Te, the Fermi level is near mid-gap at TDE, thus the possible mid-gap pinning of the Fermi level (due to interface traps) should lead to near flatband conditions. This possibility is consistent with the Ohmic contact analysis. In general, the computation of the energy band structure for nano-contacts has little sensitivity to doping level.

On the other hand, a direct mathematical fit of the experimental results to the approximated Padovani model, summarized by Eqs. (2)–(6), is straightforward. In this case the fit uses both, $N_{D,eff}$ and $\Phi_B$ as free parameters, and the results are shown in Fig. 4. This fit yields lower $N_{D,eff}$ compared to the values extracted from the calculated band structure.

Thus it was shown that the indium nano-contacts grown on two-dimensional Cd$_{0.9}$Zn$_{0.1}$Te surface exhibit asymmetric $I$-$V$ behavior. The current is negligible under positive polarity, and nearly exponential under negative bias. However, it is argued that the exponential I-V curve is the result of electron tunneling from the indium nano-contacts, while under positive polarity the overall external current is limited by the low carrier concentration in the bulk of Cd$_{0.9}$Zn$_{0.1}$Te. It is also argued that the dominance of the tunneling current does not imply that the nano-contact create a “textbook Schottky” band structure. In fact, there are plenty of evidences in the literature that macroscopic indium contacts on n-type Cd$_{0.9}$Zn$_{0.1}$Te form “Ohmic-like” contacts. Furthermore, it is shown by computer calculations that any type of contact could generate “Schottky-like” band structures under bias, when downscaled. Attempts to quantify the $J$-$V$ results by existing analytical FE model (for parabolic energy band structure) yield fair mathematical fits, but the physical meaning of the resulting fitting parameters (barrier height and doping concentration) are not yet well understood.

FIG. 3. Calculated conduction band profile of In/Cd$_{0.9}$Zn$_{0.1}$Te interfaces for two contact sizes, 10 nm and 30 nm radii.

FIG. 4. Experimental current density results fitted to field emission (one dimensional Schottky) model.