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Modelling Heating Effects due to Current Crowding in ZnO Nanowires with End-Bonded Metal Contacts

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A full 3D model for the simulation of carrier transport, self-consistently coupled with thermal transport, has been developed for free-standing ZnO nanowires with Schottky contacts. The model predicts a complex distribution of the current density through the metal-semiconductor interface with a high current density area around the edge of the Schottky contact away from the contact centre. This high current density would result in increased Joule heating at the contact edge of the free standing ZnO nanowire leading to local temperature breakdown at the contact. Degradation with increasing temperature was also demonstrated.

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1. Introduction

Thermal behaviour of metal contacts to nanostructures due to current flow has been investigated earlier in side-bonded nanostructures like graphene-metal contacts [1], ZnO, GaN [2] and SiGe [3] nanowires (NWs). These nanoscale contacts induce a current crowding effect [1] due to parasitic resistance at the edge of the downscaled contacts. Current crowding is known to result in a local temperature rise at the metal-semiconductor interface which can lead to device failure [1].

The thermal properties of the nanostructures during the current flow were studied earlier in the literature. Leonard *et al.* [3] reported the temperature distribution through the NW length with a fixed contact temperature. This simulation predicted heat loss to the environment due to the high surface to volume ratio of the NWs. LeBlanc *et al.* [2] studied the heat generation along ZnO NWs and near electrical contacts using a 1D model for the Ohmic contacts for the side-bonded ZnO NWs.

In the present work, we study the effect of current crowding on the temperature profile along the nanowire and around the metal contact for the end-bonded ZnO NWs with Schottky contacts. A full 3D model is employed in order to accurately model the geometry at the nanoscale. This 3D model considers carrier transport of electrons and holes self-consistently coupled with thermal flow [5]. The carrier transport includes both thermionic emission and tunnelling current with static dipole effects and a field dependent barrier lowering due to image force [4]. Since the transport parameters depend on the lattice temperature, lattice heating and cooling due to the carrier generation and recombination, Joule heating and Peltier-Thomson effects are also included [5]. Finally, the thermal modelling considers temperature dependent thermal conductivity model [6] and heat capacity model [7] for ZnO.

2. Simulation model

The ZnO NW is modelled with a gold end-bonded contact with a work function of 5.1 eV which creates a 0.6 eV potential barrier (ϕ_b) at the interface as calculated from the standard expression of the Schottky-Mott theory $\phi_m=\chi+\phi_b$ [8]. The image force effect and dipole effect were taken into account in the calculation of the potential barrier [9]. The thermionic emission current is calculated for both electrons and holes using a surface concentration of electrons (holes) and equilibrium concentration of electrons (holes) [10]. The universal Schottky tunneling model [11, 12] is used to calculate the tunneling current between semiconductor and metal. The tunneling current accounts for the localized tunneling rates at every grid point of the semiconductor region for both electrons and holes up to 10^{-6} cm from the metal-semiconductor interface. All quantities are calculated at each element of the triangular mesh of the structure. Dirichlet boundary conditions are used for contacts and homogeneous (reflecting) Neumann boundary conditions are used for the non-contact areas.

The effective density of states for electrons and holes, mobility and electron and hole current densities are calculated as a function of the local lattice temperature T_L. The heat flow equation[5] is used in the simulation:

$$C\frac{\partial T_L}{\partial t} = \nabla\left(k\nabla T_L\right) + H \quad (1)$$

The heat generation rate H is calculated taking into account Joule heating H_J, generation and recombination heating, and cooling H_{GR} and Thompson-Peltier effects H_{TP} as follows:

$$H = H_J + H_{GR} + H_{TP} \quad (2)$$

where

$$H_J = \left|\vec{J}_n\right|^2 \Big/ q\mu_n n + \left|\vec{J}_p\right|^2 \Big/ q\mu_p p \quad (3)$$

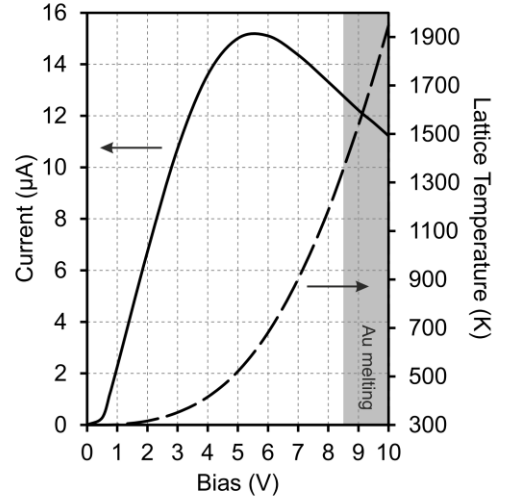

Figure 1. Simulated I-V characteristics (solid line) and a highest lattice temperature (dashed line) of the device.

$\vec{J}_n$ and $\vec{J}_p$ are the electron and hole current densities, μ_n and μ_p electron and hole mobilities, n and p are the electron and hole concentrations.

$$H_{GR} = q(R-G)\left(\left(P_p - P_n\right)T_L + \phi_p - \phi_n\right) \quad (4)$$

G and R are the carrier generation and recombination rates, P_p and P_n are the thermoelectric powers of electrons and holes, ϕ_n and ϕ_p are the quasi-Fermi levels of electrons and holes. The Thompson-Peltier effects are given by the expression:

$$H_{TP} = -T_L\left(\vec{J}_n \nabla P_n + \vec{J}_p \nabla P_p\right) \quad (5)$$

In the model, the temperature dependent heat capacitance model is used. The heat capacitance C in $J/cm^3/K$ for ZnO was approximated from experimental data [7] as a function of the lattice temperature as follows:

$$C = 3.22 + 4.68\cdot10^{-4}T_L - 1.31\cdot10^{-8}T_L^2 - 4.74\cdot10^4 T_L^{-2} \quad (6)$$

The thermal conductivity k in $W/cm\cdot K$ for ZnO was approximated from experimental data [13] using a temperature-dependent power model:

$$k(T_L) = 0.37\big/(T_L/300)^{1.53} \quad (7)$$

The thermal boundary condition with the fixed temperature of 300 K is specified at the bottom contact of the structure, and an air region around the structure is used as a heat sink layer in the calculations.

3. Current Crowding

A complex spherical Au particle shape observed in experiments [14] was used in the simulations of free standing ZnO nanowires with end-bonded Schottky contacts (Fig. 2). Transmission electron microscopy (TEM) images of the ZnO-Au structure [14] indicate a complex shape of the Au particle standing on the top of the nanowires of various radius. To have a good geometrical representation of the structure in the simulations, we mimic the shape from images of the Au particle where the interface radius is 80-90% smaller than the Au particle radius [14]. A 15 nm radius of the Au particle was approximated using 4 large cylindrical layers. An 80% change in the particle at the base of the contact was approximated using 3 cylindrical sublayers (Fig. 2). The NW length of 900 nm was assumed in all simulations. The following material parameters were used for ZnO[15]: band gap (E_g) 3.37 eV, electron affinity (χ) 4.5 eV, and *n*-type doping of 10^{18} cm^{-3} assuming a gold work function (ϕ_m) of 5.1 eV.

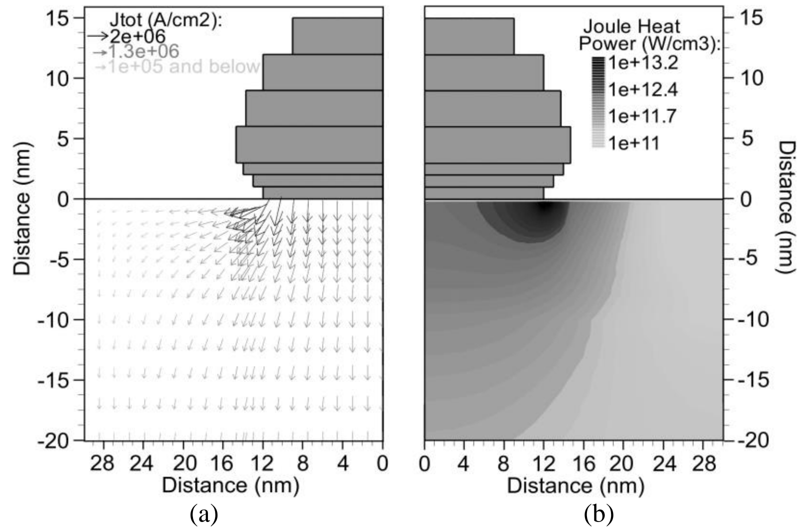

Figure 2. (a) Schematic plot of the current vectors near the contact edge at 8 V demonstrating the current crowding effect. (b) Spatial distribution of the Joule heating power at 8 V.

The simulation results in Fig. 1 demonstrate the current decrease at around 5 V due to the high generation of Joule heating near the contact. As the device temperature is further increased with the increased voltage until ~8.5 V, the Au contact melting temperature is reached which can lead to device failure. In Fig. 2(a), the current vectors indicate the increased current density at the edge of the contact. Due to the local thinning of the potential barrier at the corners of the Au contact, the current transport will mostly occur through the narrow region at the contact edge and will result in the local current crowding effect. The increased current density will lead to the high Joule heat generation at the edge of the contact as shown in Fig. 2(b). As a result the spatial distribution of the temperature at 8 V bias in Fig. 3 indicates the higher local temperature around the NW contact up to nearly 1200 K.

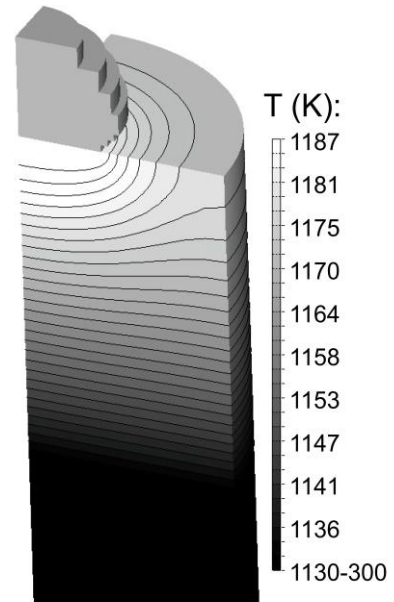

Figure 3. Spatial distribution of the lattice temperature at 8 V (only the top of ~70 nm of the nanowire length is shown).

4. Conclusion

The full 3D model was implemented for the thermal calculation of the free-standing ZnO nanowires with the end bonded contacts. Simulation predicts that due to the complex

geometry of the end-bonded ZnO nanowires the effect of the current crowding will happen around the metal contact at the edge of the contact. This will lead to a significant heat generation with a rise of the local temperature up to 1337 K which will result in device failure due to the contact melting. This identifies the need to engineer the contacts to reduce the barrier thinning near the contact edges, or use a method to allow generated heat to flow away from the interface more efficiently.

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