Temperature- and doping-dependent nanoscale Schottky barrier height at the Au/Nb: SrTiO$_3$ interface

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We use ballistic electron emission microscopy to investigate prototypical Au/Nb-doped SrTiO$_3$ (NSTO) Schottky barrier diodes for different temperatures and doping levels. To this end, ultrathin Au overlayers are thermally evaporated onto TiO$_2$-terminated NSTO single crystal substrates. We show that at room temperature, regardless of the nominal doping, rectification is controlled by a spatially inhomogeneous Schottky barrier height (SBH), which varies on a length scale of tens of nanometers according to a Gaussian distribution with a mean value of 1.29–1.34 eV and the standard deviation in the range of 80–100 meV. At lower temperatures, however, doping effects become relevant. In particular, junctions with a low Nb content of 0.01 and 0.05 wt. % show an ∼300 meV decrease in the mean SBH from room temperature to 80 K, which can be explained by an electrostatic analysis assuming a temperature-dependent dielectric permittivity for NSTO. In contrast, this model fails to predict the weaker temperature dependence of SBH for junctions based on 0.5 wt. % NSTO. Our nanoscale investigation demands to reassess conventional models for the NSTO polarizability in high-intensity electric fields. Furthermore, it contributes to the comprehension and prediction of transport in metal/SrTiO$_3$ junctions and devices.

Fig.1: (a) Schematic diagram of the Au/NSTO junction and the experimental setup for BEEM measurements. (b) STM topography and (c) BEEM map acquired simultaneously over a representative Au region (I$_{IT}$= 45 nA, V$_T$ = −1.85 V, T = 291 K, x$_{Nb}$=0.01 wt.%). The arrows highlight a few localized grains with high BEEM contrast.

Fig.2: Representative raw spectra acquired at different temperatures on Au/NSTO junctions. (c) Dual parameter ($\Phi_B$, $R$) distributions (top) and $\Phi_B$ histograms (bottom) for x$_{Nb}$=0.01 wt.% The average SBHs at 291 K (1.34 eV) and 80 K (1.07 eV). (d) as in (c) but for x$_{Nb}$=0.5 wt.%.

Fig.3: (a) Temperature dependence of the spatially averaged SBH $\Phi_B$ measured by BEEM for Au/NSTO junctions with two different doping levels. The solid and dashed lines are theoretical predictions with the metal-insulator-semiconductor (MIS) model. (b) Schematics of the energy band diagram for the low-doped unbiased junction (not in scale).