A Transport Analysis of the BEEM Spectroscopy of Au/Si Schottky Barriers

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(January 2, 2018)

Abstract

A systematic transport study of the ballistic electron emission microscopy (BEEM) of Au/Si(100) and Au/Si(111) Schottky barriers for different thicknesses of the metal layer and different temperatures is presented. It is shown that the existing experimental data are compatible with a recently predicted bandstructure–induced non–forward electron propagation through the Au(111) layer.

PACS: 61.16 Ch, 72.10 Bg, 73.20 At.

REF.: Phys. Stat. Sol. (b), submitted.

I. INTRODUCTION

Ballistic-electron emission microscopy (BEEM) has proven to be an extremely efficient tool to study metal-semiconductor interfaces on a nanometer scale \cite{1,2}. BEEM is a technique based on scanning tunneling microscopy (STM) where the STM tip is used as an electron source for a highly space–resolved injection into the metal layer. By collecting the current which passes from the metal into the semiconductor as a function of tip position and tip bias, information about the local Schottky barrier height and the hot-electron transport properties can be obtained on a nanometer scale.

Although the Au/Si interfaces have been among the systems most thoroughly studied with the BEEM technique, they also turned out to be among the most controversial ones. In particular, the very similar BEEM spectra for Au/Si(100) and Au/Si(111) systems \cite{3} have been a matter of intensive debate \cite{4}. A number of theoretical models has been brought up to account for these experimental findings. While these models have been successful in the interpretation of particular systems, only few attempts have been reported to explain the various experimental data with just one model. The goal of the present $\vec{k}$–space analysis is to provide a transport model that improves on the hitherto used energy–space descriptions in two important ways. First, we explicitly take into account that in the Au(111) layer no propagation is allowed along the (111)-direction. Second, our scattering dynamics contains no adjustable parameters.
II. THEORETICAL MODEL

Our transport model is based on the semiclassical Boltzmann equation which is solved in \( \vec{k} \)-space by use of the Ensemble–Monte-Carlo (EMC) technique [5].

A recent Green–function analysis [4] has shown that the STM electrons achieve their bulk Bloch character, with propagation gaps due to forbidden regions of phase space, after passing roughly 50 Å within the Au(111) layer, with the asymptotic form \( \sim 1/\cos \theta \) and \( \theta \in (20^\circ, 70^\circ) \); this distribution differs appreciably from the hitherto assumed distribution for an isotropic bandstructure which is concentrated within a narrow forward cone. As the mean free path of the injected electrons in the gold layer is usually larger than 50 Å, our EMC simulations use the asymptotic angular distribution for the input ensemble of injected STM electrons at the surface. Simulating quasifree electrons \( (m_{\text{ef}} = m_o) \), we approximately correct for band-structure effects of the electron propagation by cutting off the forbidden directions arising from gaps in the constant-energy surface. For our case of injection energies about 1 eV above the Fermi energy, these "propagation gaps" form cones with an opening angle of 10 degrees around the (111) directions and are included in the scattering dynamics by use of Monte-Carlo rejection techniques. The scattering between the hot electrons and those of the "cold" metallic background is treated via a dynamically (in RPA) screened Coulomb potential, and the electron-phonon scattering with an experimentally determined acoustic deformation potential [6].

Assuming specular transmission/reflection at the Au/Si interface (via wavefunction matching at a step-like Schottky barrier of 0.8 eV) and either specular or diffuse reflection of backward–running electrons at the free metal surface (both types resulting in practically identical simulated BEEM currents), the boundary scatterings are treated in the conventional way [2].

The simulation of each electron is followed in \( \vec{k} \)- and \( \vec{r} \)-space and stopped after it has passed the interface or when its energy has dropped below the top of the barrier. Finally, we assume negligible current modifications in the semiconductor, which seems reasonable for the modest electron energies of our present concern.

III. RESULTS

Our simulated Au/Si(111) BEEM spectra compare reasonably well with those in Fig.1 of Ref. [7], with the exception of the 300Å sample at 77 K where our simulations completely fail to reproduce the experimental finding of a drastically altered shape and magnitude [8] (see also symbol ⋄ in our Fig.1). We note that for its interpretation Bell [7] had proposed a model based on a narrow forward injection cone, i.e. propagation inside the forbidden gaps.

To further inquire into this problematics we compare in Fig. 1, for a constant tip voltage of 1.2 V, our theoretical results (using a tunneling distribution of energetic width 0.5 eV) with various experimental BEEM data [7,10,3,9,12–14]. Good agreement with the experimental trends is found, e.g. (i) for Au/Si(100) the BEEM current at 77 K is always larger than the current at room-temperature, (ii) for almost all experimental data the BEEM current for Au/Si(100) is larger than the current for Au/Si(111).

We emphasize that a number of important ingredients is still missing in our transport description, as e.g. phonon–induced backscatterings in the image–charge potential region...
of Si [10], effects of the non-isotropic band structure on the scattering dynamics, a possible mismatch of the in-plane $\vec{k}$-vector at the interface [2], more pronounced anisotropies of the injected electron distribution, and non-ideal tip-surface geometries [11]. Nevertheless, the fact that our parameter-free calculations yield qualitative agreement with the (widely scattered) experimental data gives us confidence in our approach.
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FIG. 1. Transmittance of the Au(111)/Si interface at a tunnel voltage of 1.2 eV as function of the Au–layer thickness.