<table>
<thead>
<tr>
<th><strong>Title</strong></th>
<th>Calculation of Cu/Ta interface electron transmission and effect on conductivity in nanoscale interconnect technology</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Author(s)</strong></td>
<td>Feldman, Baruch; Dunham, Scott T.</td>
</tr>
<tr>
<td><strong>Publication date</strong></td>
<td>2009</td>
</tr>
<tr>
<td><strong>Type of publication</strong></td>
<td>Article (peer-reviewed)</td>
</tr>
</tbody>
</table>
[http://dx.doi.org/10.1063/1.3257700](http://dx.doi.org/10.1063/1.3257700)  
Access to the full text of the published version may require a subscription. |
| **Item downloaded from** | [http://hdl.handle.net/10468/4348](http://hdl.handle.net/10468/4348) |

Downloaded on 2019-01-08T20:41:49Z
Calculation of Cu/Ta interface electron transmission and effect on conductivity in nanoscale interconnect technology

Baruch Feldman and Scott T. Dunham

Citation: Appl. Phys. Lett. 95, 222101 (2009); doi: 10.1063/1.3257700
View online: http://dx.doi.org/10.1063/1.3257700
View Table of Contents: http://aip.scitation.org/toc/apl/95/22
Published by the American Institute of Physics

Articles you may be interested in

Simulation of junctionless Si nanowire transistors with 3 nm gate length
Applied Physics Letters 97, 062105 (2010); 10.1063/1.3478012

Dependence of resistivity on surface profile in nanoscale metal films and wires

Alteration of Cu conductivity in the size effect regime
Calculation of Cu/Ta interface electron transmission and effect on conductivity in nanoscale interconnect technology

Baruch Feldman1,a) and Scott T. Dunham1,2

1Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA
2Department of Electrical Engineering, University of Washington, Seattle, Washington 98195-2500, USA

(Received 21 July 2009; accepted 9 October 2009; published online 30 November 2009)

Resistivity augmentation in nanoscale metal interconnects is a performance limiting factor in integrated circuits. Here we present calculations of electron scattering and transmission at the interface between Cu interconnects and their barrier layers, in this case Ta. We also present a semiclassical model to predict the technological impact of this scattering and find that a barrier layer can significantly decrease conductivity, consistent with previously published measurements. © 2009 American Institute of Physics. [doi:10.1063/1.3257700]

As the minimum feature size in transistors continues to shrink, nanoscale metal wires with thickness $\leq 32$ nm will soon be needed to interconnect transistors in integrated circuits. However, measurements show nanoscale metallic wires have substantially higher resistivity than bulk metals,\textsuperscript{1-3} leading to performance-limiting interconnect delays and power dissipation.\textsuperscript{3} Scattering from rough wire surfaces, interfaces with liner layers, and grain boundaries are believed to be the causes of this conductivity degradation,\textsuperscript{3} but microscopic understanding of these effects and quantitative predictions of their magnitude have been limited. In recent articles, we have considered scattering from surfaces\textsuperscript{4} and grain boundaries,\textsuperscript{5} and in this letter, we present calculations of scattering and transmission at the interface between Cu interconnects and their liner layers.

Nanoscale Cu wires in integrated circuits are surrounded on three sides by a liner layer, typically made of Ta, TiN, or Ti. Also known as a barrier/adhesion/seed layer, this layer acts as a seed for the deposition of Cu, improves adhesion of the Cu to the sidewalls, and prevents diffusion of Cu into the dielectric. To inhibit the migration of Cu atoms, the liner layer is made of a refractory metal with small lattice mismatches and poor conductivity despite being metallic. In this letter, we consider for the liner layer the most common form of Ta when deposited epitaxially on Cu, $\beta$-Ta\textsuperscript{6-8}, which has a bulk resistivity of $(200\pm20)\ \mu\Omega\cdot\text{cm},$\textsuperscript{6,8,9} compared to 1.7 $\mu\Omega\cdot\text{cm}$ for Cu.

$\beta$-Ta (Refs. 7 and 9) has a tetragonal lattice with dimensions $a=10.2$ Å and $c=5.3$ Å. In the [002] direction (corresponding to the $c$ lattice parameter), it contains four equally spaced layers, which consist of either four regularly spaced Ta atoms or 11 atoms arranged in a pseudohexagonal pattern. The $\beta$-Ta unit cell contains a total of 30 atoms. Simulations\textsuperscript{10} and measurements\textsuperscript{5} indicate that for Cu deposited on a (002) $\beta$-Ta liner layer, the $\beta$-Ta matches heteroepitaxially to Cu (111) surfaces with a relative strain in each $a$ direction of approximately 7%, causing the pseudohexagons in Ta to match those in the Cu (111) planes.

We have set up such an epitaxial simulation cell for relaxation with the VASP density functional theory (DFT) code.\textsuperscript{11} Our interface contains a total of 56 Ta and 64 Cu atoms with periodic boundary conditions in the plane of the interface (Fig. 1). These boundary conditions are made realistic by the epilayer relationship, which should impose rough periodicity over actual interfaces. As shown in Fig. 1, our Ta region terminates with an 11-atom Ta layer, interfacing with a partial Cu layer with four atoms, followed by four full (15-atom) Cu (111) layers. We considered a range of interface structures, and this gave the lowest energy. We relaxed this system within DFT, keeping the bottom Ta layer fixed and allowing the top Cu layer to adjust only in the $z$ dimension. This allowed the interface $z$-spacing to relax. The variation in $z$-position among Cu atoms within the topmost layer after relaxation was very small compared to the layer spacing.

To simulate transmission across a Cu/Ta interface, we replaced $z$-coordinates of the topmost Cu layer by their average, leaving ideal Cu and ideal strained $\beta$-Ta layers bounding the interface region. We then set up a transmission simulation across the interface, using the relaxed interface of Fig. 1 as a scattering region and matching the perfect Cu and Ta layers to electrodes made of ideal lattice vectors of the respective materials. We used the code ATOMISTIX\textsuperscript{12} to perform non-equilibrium Green’s function method\textsuperscript{13} simulations of dynamical transmission across interfaces, as in our previous article.\textsuperscript{5}

In this formulation, transmission probability is given by

$$T = \frac{T_{\bar{e}}}{M},$$

where $T_{\bar{e}}$ is the transmission (conductance in units of $2e^2/h$) and $M$ is the Sharvin conductance in units of $2e^2/h$, which is equal to the number of current-carrying modes.\textsuperscript{13} Note that conduction electron density, and therefore $M$, is different in the two materials. We obtained $M$ for (002) strained $\beta$-Ta and (111) Cu by separate transmission simulations, finding a ratio $M_{\text{Cu}}/M_{\text{Ta}}=1.8$. However, reciprocity requires that $T$ is the same for transmission in either direction across the interface,\textsuperscript{13} so the net current is zero across the unbiased interface after the vacuum levels have adjusted to equilibrate the Fermi levels.\textsuperscript{14} We calculated $T$ for transmission from Ta to Cu only, using the $M$’s to find an overall transmission probability $T=0.22$ for electrons originating in Cu and 0.39 for those originating in Ta.

Let us consider the effect on conduction of transmission across the interface. Although the liner layer represents a parallel conductance to the Cu wire, the high resistivity of

\textsuperscript{a)Present Address: Tyndall National Institute, University College Cork, Cork, Ireland. Electronic mail: baruchf@alum.mit.edu.}
\[ \frac{\rho}{\rho_b} = 1 + \frac{3\lambda P}{16A}(1-p), \]

for arbitrary cross section, where \(1-p\) is the proportion of electrons that lose their momentum on interaction with the surface. In our case, this is the proportion of electrons transmitting into the barrier layer and losing their net drift velocity before returning to Cu.

The assumption of zero drift velocity for returning electrons is valid when the Ta thickness is large compared with the bulk mean free path \(\lambda_{Ta}\) in \(\beta\)-Ta, which we estimate as follows. The product of Sharvin (ballistic) conductance and bulk resistivity gives a length scale of order the bulk mean free path,\(^13\) a relation that holds to within 40\% for Cu.\(^18\) For strained (002) \(\beta\)-Ta, our calculation of \(M_{Ta}\) combined with bulk resistivity measurements suggest \(\lambda_{Ta} \sim 1\) nm (compared to \(\lambda = 39\) nm in Cu).

We now combine Eq. (2) with our calculated transmission probability to find the effect on conductivity from scattering in the barrier layer. Treating transmission into Ta as equivalent to a diffuse scattering event, the effective \((1-p)\) for a wire would be given by

\[ 1 - p_{\text{line}} = (1 - p_s) \frac{P - P_i}{P} + \left\{ 1 - p_i + T \right\} \frac{P_i}{P}, \]

where \(P\) is the total wire perimeter and as in Eq. (2), \(P_i\) is the perimeter interfacing with the liner layer, \(1 - p_i\) is the diffuse reflection probability from the Cu/Ta interface, and \(1 - p_s = 0.04\) is our previously calculated diffuse probability for a rough Cu surface.\(^4\) Here we will use \(p_s = p_i\) as a crude approximation. Equations (2) and (3) give a resistivity augmentation of about 13\% for a 45 nm Cu square wire surrounded by Ta of more than about 2 nm on three sides, and 4\% for a 45 nm Cu film with Ta on one surface.

We can also easily extend this analysis to consider thinner liner layers of thickness \(t_{Ta}\). The cumulative scattering probability is Poisson

\[ P(s) = 1 - e^{-s/\lambda}, \]

where \(s\) is distance traveled and \(\lambda\) is mean free path. Then the probability that an electron leaving Ta scattered since coming from Cu is given in terms of the transmission probability from Ta, \(T_{Ta} = \bar{T}/M_{Ta}\), by

\[ 1 - e^{-2t_{Ta}/\lambda_{Ta}} \sum_{n=0}^{\infty} \left\{ e^{-2t_{Ta}/\lambda_{Ta}}(1 - T_{Ta}) \right\}^n \]

\[ = \frac{1 - e^{-2t_{Ta}/\lambda_{Ta}}}{1 - (1 - T_{Ta})e^{-2t_{Ta}/\lambda_{Ta}}}, \]

(Here \(n\) is the number of internal reflections within Ta, which each occur with probability \(1 - T_{Ta}\)). So we find

\[ 1 - p_{\text{line}}(t_{Ta}) = (1 - p_s) \frac{P - P_i}{P} + \left\{ 1 - p_i \right\} \left\{ \frac{1 - e^{-2t_{Ta}/\lambda_{Ta}}}{1 - (1 - T_{Ta})e^{-2t_{Ta}/\lambda_{Ta}}} \right\} \frac{P_i}{P}, \]

which interpolates smoothly between our surface scattering-only result and Eq. (3). Here \(T_{Cu} = \bar{T}/M_{Cu}\) is the transmission probability from Cu.
The form of Eq. (4) agrees qualitatively with the results of Rossnagel and Kuan, who measured sheet resistance of a 45 nm Cu film with 0–5 nm of Ta deposited on it (note they use a film and deposit Ta on only one surface). They find resistivity augmentation rapidly increasing by 10% for overlayer thickness, as measured in Ref. 15. Also shown are fits to Eq. (4), with $T_{Cu}$ at our calculated value of 0.22 as well as a better fit value of 0.54. See discussion in the text regarding this quantitative discrepancy.

The form of Eq. (4) agrees qualitatively with the results of Rossnagel and Kuan, who measured sheet resistance of a 45 nm Cu film with 0–5 nm of Ta deposited on it (note they use a film and deposit Ta on only one surface). They find resistivity augmentation rapidly increasing by 10% for overlayer thickness, as measured in Ref. 15. Also shown are fits to Eq. (4), with $T_{Cu}$ at our calculated value of 0.22 as well as a better fit value of 0.54. See discussion in the text regarding this quantitative discrepancy.

Increasing Cu sheet resistance as a function of Ta overlayer thickness, as measured in Ref. 15. Also shown are fits to Eq. (4), with $T_{Cu}$ at our calculated value of 0.22 as well as a better fit value of 0.54. See discussion in the text regarding this quantitative discrepancy.

FIG. 2. (Color online) Increasing Cu sheet resistance as a function of Ta overlayer thickness, as measured in Ref. 15. Also shown are fits to Eq. (4), with $T_{Cu}$ at our calculated value of 0.22 as well as a better fit value of 0.54.

We would like to thank Thomas Pedersen and Dmitri Novikov for helpful discussions. This work was supported by Intel Corporation.

14. A space charge region must form at the interface, analogous to that at a PN-junction, to bring about this equilibrium.
18. Semiclassically, one can think of an electron traveling ballistically in between bulk scattering events.