Analysis of Surface Roughness Scattering and Its Contribution to Conductivity Degradation in Nanoscale Interconnects

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Abstract

We use a quantum mechanical calculation of momentum loss rates as function of spatial frequency of surface roughness to identify which frequencies contribute most strongly to conductivity degradation. We combine these calculations with surface roughness spectrum from atomic step model matched to AFM data. We find that roughness with period on the order of 300nm gives greatest contribution to resistance increase, but that scattering from typical Cu surfaces can be expected to be nearly specular. We attribute apparent surface scattering to adhesion/barrier layer properties rather than interface or surface roughness.

Introduction

High performance nanoscale interconnects are required for connecting arrays of future nanodevices, whether they are conventional MOS transistors or an alternative technology. However, experimental studies on metal nanowires have found substantial increases in resistivity for wire dimensions below 100nm [1,9], which have been attributed to surface and grain boundary scattering.

Most quantitative treatments of surface and size effects on the transport properties of thin films or wires have been based on semiclassical methods via solution of the Boltzmann equation as in work of Fuchs [2] and Sondheimer [3]. In these models, an empirical specular scattering fraction p ($0 \le p \le 1$) is chosen for a surface to fit experiment result, with the remainder of surface scattering assumed to be diffuse

As semiconductor technology has entered the sub-100nm regime, the significance of conductivity decrease has raised the concern of researchers in industry [4,5]. Theoretical physicists have also proposed several quantum mechanical approaches to account for the contribution of quantum confinement to conductivity degradation in nanoscale structures. One approach is Kubo linear response theory, where total conductivity is given by a sum of conductivity of all subbands [6]. An alternative is the diagrammatic Keldysh formalism [7] in which intersubband transition can also be taken into account.

In this paper, we will follow the latter approach because we are interested in the 10-100nm size scale, for which there are a large number (100 to 1000) of closely spaced electron subbands and transitions between subbands are important. Using this method, we evaluate the contributions of different spatial frequencies of the surface roughness to momentum loss in directions parallel to surface and combine these results with surface roughness spectrums to predict resulting impact on conductivity in thin films.

Theoretical Approach

We consider a film of thickness L as in Fig. 1 with random rough boundaries at

$$x = -L/2 - \xi_1(y,z) \qquad x = L/2 + \xi_2(y,z).$$

Given potential $U(x)$ for flat interface and with ξ small, the potential $U(x+\xi)$ on the corrugated surface can be taken as

$$U(x+\xi) = U(x) + \xi \partial U/\partial x$$

with $\partial U/\partial x = U(\pm L/2)\delta(x \mp L/2)$, for abrupt change in potential at the boundaries.

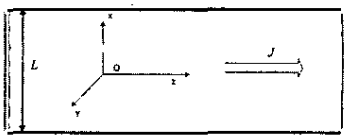

Fig.1 System and coordinate setup. J indicates the direction of current flow.

The surface roughness can be described by correlation function for the relative surface height. The correlation function and its Fourier transformation (also called power spectrum) are defined as

$$\zeta(|\mathbf{s}|) = \langle \xi(\mathbf{s}')\xi(\mathbf{s}'+\mathbf{s}) \rangle \equiv A^{-1} \int \xi(\mathbf{s}')\xi(\mathbf{s}'+\mathbf{s}) d\mathbf{s}'$$

$$\zeta(|\mathbf{q}|) = \int d^2 s e^{i\mathbf{q}\cdot\mathbf{s}} \zeta(|\mathbf{s}|) = 2\pi \int \zeta(|\mathbf{s}|) J_0(qs) s ds \qquad (1)$$

$$\mathbf{s} = (y,z), \mathbf{q} = (q_y, q_z)$$

The scattering matrix elements can be calculated from unperturbed wave functions (subband wave functions in this case) as,

$$V_{ij} \equiv \langle i | \xi \partial U/\partial x | j \rangle$$

$$= \int \exp[i\mathbf{s}\cdot(\mathbf{q}-\mathbf{q}')\xi(\mathbf{s})\psi_i U(L/2)\delta(x-L/2)\psi_j d\mathbf{s}dx].$$

Transition rates are just simply given by $|V_{ij}|^2$ and thus are quadratic in the power spectrum of roughness. With these transition rates, Waldmann-Snider transport equations under the relaxation time approximation [7] give conductivity change due to surface scattering. Assuming the transition rate matrix between sub-bands is almost diagonal, the

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conductivity is equal to [7]

$$\sigma = \frac{2e^2L^2}{3\hbar^3}\sum_j \frac{q_j^2}{(\frac{\pi j}{L})^4 \sum_{j'} \zeta_{jj'}^{(0)} (\frac{j'}{j})^2 - \zeta_{jj}^{(1)}} \quad (2)$$

However, when interband scattering is dominant or precise results are preferable, the linear equations must be solved numerically to obtain accurate conductivity value.

Results and Discussion

We analyzed the effect of narrow-band (single frequency) roughness on momentum loss due to surface scattering using Equation (2). The aim of this analysis is to answer an important question for technology development: which components of power spectrum of surface roughness have the greatest influences on conductivity? With this knowledge, we can focus process development efforts to reduce the most critical components of surface roughness.

We assume surface roughness is isotropic and consider surface roughness limited to spatial frequencies with magnitude k. We need the zeroth and first order angular harmonics to find conductivity. For this delta function power spectrum, the first and second harmonics are,

$$\zeta^{(0)} = \frac{1}{\pi}\int_0^{2\pi} \delta(\sqrt{q^2+q'^2-2qq'\cos\chi}-k)d\chi = \frac{qq'\sin(\chi)}{\pi\sqrt{q^2+q'^2-2qq'\cos\chi}}$$

$$\zeta^{(0)} = \frac{1}{\pi}\int_0^{2\pi} \delta(\sqrt{q^2+q'^2-2qq'\cos\chi}-k)\cos\chi d\chi = \frac{qq'\sin(\chi)\cos(\chi)}{\pi\sqrt{q^2+q'^2-2qq'\cos\chi}}$$

with

$$\cos(\chi) = \frac{k^2-(q^2+q'^2)}{2qq'}, \sin(\chi) = \sqrt{1-\cos^2(\chi)}$$

q, q' depend on j, j', the initial and final subbands.

From Equation (2), conductivities as function of magnitude of spatial frequency of roughness were calculated for two different film thicknesses in the absence of bulk scattering, and the corresponding momentum loss rates calculated from $1/\tau_p = ne^2/m\sigma$. Results are shown in Fig. 2. The momentum loss rate increases with increasing spatial frequency due to the larger change in momentum upon scattering and changes in the available density of states. As expected from classical picture, the thicker film gives a lower momentum loss rate in inverse proportion to film thickness.

Experimental data on the surface roughness spectrum of metal films or wires is very limited in the literature and tends to focus on relatively large length scales. To bridge this gap, we used an atomic surface step model to generate surfaces (and associated roughness spectrums) that we can compare to available experiment. We consider a model for surface roughness in one dimension (like an atomic chain) starting with an atom at height h. The next surface atom has a probability $\beta-\xi\cdot\alpha$ to be one atomic layer higher (α, β are parameters), a probability $1-2\beta$ to stay at the same level and a probability $\beta+\xi\cdot\alpha$ to be lower. This simple algorithm generates a series of integers representing a one-dimensional rough surface.

We have compared the results of this approach with published experiment data for Cu films [8] by choosing appropriate parameters for step frequency β and spring constant α as shown in Fig. 3. The aim of this effort was to test and characterize the roughness model by comparison to the data and then use the simulated results to extrapolate to higher spatial frequencies, which have a particularly significant impact on the interface scattering effectiveness (see Fig. 2). In these simulations, RMS roughness of the surface is controlled by ratio of step frequency to spring constant (retraction modulus), which biases up/down step frequency to bring thickness back to mean value. Other more extreme values for parameters have been also tried. Although they result in differences in the lower frequency region, the higher frequency portion of the curves have same slope as the three curves shown in Fig. 3. We suspect that the more rapid

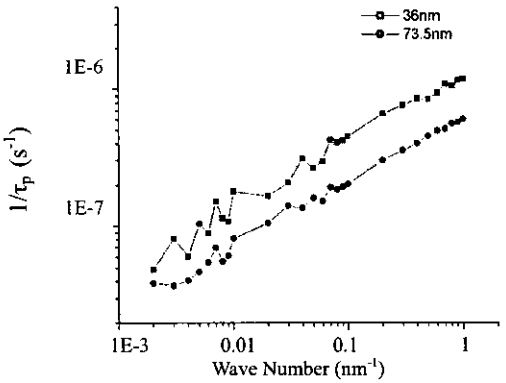

Fig. 2 Momentum loss rates due to surface roughness versus magnitude of spatial frequency.

fall-off in experimental results may be due to the finite size of the AFM tip attenuating smaller features. The difference observed would be consistent with a tip radius on the order of

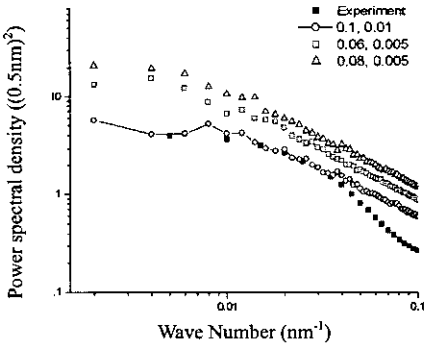

Fig. 3 Comparison of surface roughness from random walk simulations to experiment data for copper films measured via AFM [8].

30 nm. Note that the flattening near the highest frequency is due to the finite sampling interval used in experiment. Due to the potential importance of the roughness range near and above $0.03nm^{-1}$, it would be very useful to try to measure roughness on this scale using STM and/or AFM with carbon nanotube tips.

If we consider surface roughness spectrum shown in Fig. 3, we can identify which portion of the surface roughness spectrum is most important to conductivity by convolving the

surface roughness spectrum predicted by random step model matched to experimental data with the momentum loss versus frequency. The result is that the most important contribution to conductivity degradation is due to surface roughness with spatial frequencies around $0.02nm^{-1}$, which corresponds to period of about 300nm. This reflects that although diffuse scattering is strongest for high spatial frequencies, these frequencies tend to have much lower RMS magnitudes, with the surface roughness spectrum falling off more strongly with frequency than the increase in momentum loss rate.

Finally, we check the effective surface specular scattering ratio predicted by this calculation (p in models of Fuchs and Sondheimer. [2,3]). Using the roughness spectrum of Ref [8], we get a specular scattering fraction of 0.99, almost totally specular. For a larger surface fluctuation magnitude of 7nm, the specular ratio is calculated to be 0.93, which means that even with a relatively rough surface, surface roughness has little contribution to overall conductivity degradation.

These results can interpreted in light of recent measurements by Rossnagel et al [10], who examined the change of film conductivity associated with deposition and then oxidation of ultrathin Ta layer on Cu film. They found that the conductive Ta layer significantly raised the sheet resistance (despite adding to thickness), but upon exposure to atmosphere resulting in reaction to form insulating Ta-oxide, the conductivity degradation was reversed. The change in resistance was consistent with a change in specular ratio p of top surface from near 1 to 0.6 and back. The system analyzed in this paper is equivalent to a rough metal/insulator interface for which there is a sharp increase in electron potential, and our results indicate that scattering for this case should be primarily specular. In contrast, there is no barrier for

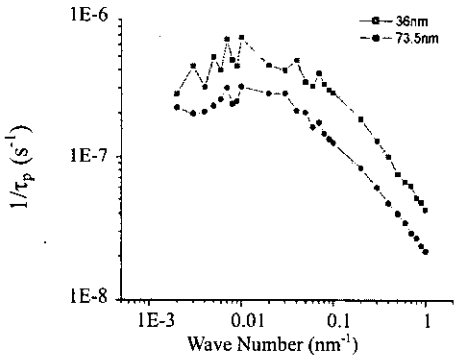

Fig. 4 Momentum loss rates versus magnitude of spatial frequency of after convolution with surface roughness spectrum of random-walk model.

penetration of electrons into Ta surface layer. Since Ta (as with most barrier/adhesion layers) is a high temperature material, it is deposited with high levels of disorder, which may lead to substantial diffuse scattering. Alternatively, Rossnagel et al [10] have suggested that the strong diffuse scattering is due to Fermi surface mismatch between Cu and Ta. These results suggest that changes in barrier/adhesion layers (e.g., use of crystalline layers or insulating layers such as SiC [11] when possible) may allow scaling of Cu nanowires with minimal resistivity degradation if nanowires can be fabricated with large grain sizes to minimize grain boundary scattering [12].

Conclusion

We conducted quantum mechanical calculations of conductivity degradation due to random rough surfaces. We separated out the effects of varying spatial frequencies of the roughness, so that the results could be applied easily to surfaces with arbitrary roughness spectrums. We found that momentum loss in plane parallel to surface was largest for higher spatial frequencies. By convolving these results with the actual surface roughness spectrum, we are able to calculate the resistivity increase due to surface scattering. Because of limited data for roughness versus frequency of Cu films/wires at high spatial frequencies, we developed a random step simple model for estimating the variation of roughness magnitude with frequency. Considering both the surface roughness spectrum and the momentum loss rate versus frequency, we find that roughness with period on the order of 300nm dominates momentum loss. However, we find that actual amount of diffuse scattering small for typically smooth Cu surfaces, and attribute the degradation of resistivity with size to be due to scattering in adhesion/barrier layers and/or at grain boundaries.

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