Investigation of Contact Resistance and Aluminum Spiking during NiSi Nickel Mono-Silicide formation

Mark Zimmerman

Advisor: Paul Berger

Graduate Student Mentor: Ronghua Yu

The Ohio State University, Columbus, Ohio

Low-resistivity NiSi formation, and its reduction of the contact resistance at a metal-semiconductor interface are observed by simple rapid thermal annealing at 430° C for 60 seconds with metal Al pads already in place above the Ni, on the Si substrate. Specific contact resistivity measurements obtained varied with initial substrate doping concentration, but the lowest number obtained was 4.42 E-6 Ω cm^2. Diodes were created with the Ni-Al structure on one side to test the severity of Al spiking, and these diodes were observed to be destroyed with anneals as small as 450° C for 30 seconds. Attempts to place a barrier layer between Ni and Al to hold the spiking at bay were unsuccessful.

I. INTRODUCTION

Continually decreasing device sizes and increasing devices numbers have made contact resistance an increasingly important issue in the computer industry. Contacts must be obtained that have both very ohmic behavior and low resistance. A structure suitable for these requirement which has previously been studied is silicide, a low-resistivity compound that forms between silicon and several metals. The concern of this paper focuses on NiSi, the low-resistivity form of nickel silicide, which forms in a temperature range of approximately 400-800° C.[1] The sheet resistivity of NiSi has been cited in the range of 3 Ω/ÿ.[2]

Since silicide is very brittle, in order to contact electrically with it a pad of metal must be placed on top of it. This allows for interconnects between devices or contacts with them using probe needles. Aluminum has been widely used in the field and is a very cost-friendly material, and so it will be used for this purpose here.

Aluminum brings with it some of its own difficulties, however. Aluminum, like many metals, is reactive with silicon itself, and so the concentration gradient between them causes for Al diffusion into silicon during annealing to be uneven and extreme: hence Al spiking. We sought here to determine whether or not spiking was on a serious enough scale to reach down to the active layers of the silicon, causing damage to or destroying the devices contained therein, and if so, to evaluate two possible materials as barrier layers to Al spiking: Chromium and Molybdenum. These metals were chosen for their high melting points, hoping their structure would remain in tact enough to hold the Al at anneal temperatures.

II. THEORY

Metal-semiconductor contacts have an intrinsic resistance to the flow of charge across their junction, and this is known as the Schottky barrier. This barrier is often not symmetrical – it is also the source of the behavior of the Schottky diode, the rectifying behavior that is undesirable when trying to manufacture ohmic contacts. The barrier arises from the difference in Fermi level energy between the two, and the necessary lining up of Fermi levels that occurs at the junction.

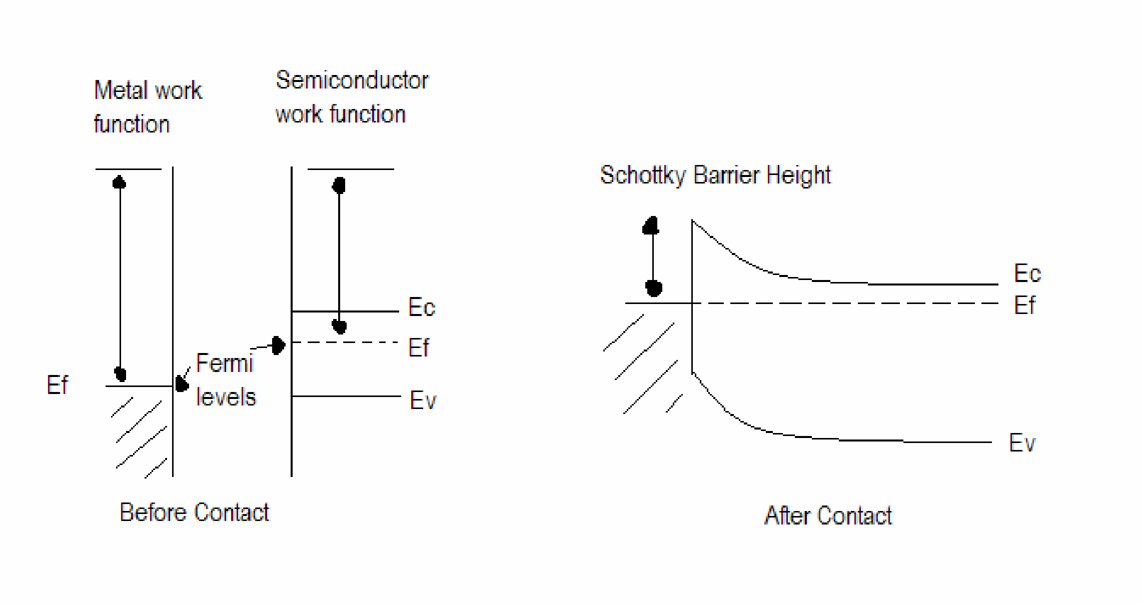

Figure 1 – Creation of the Schottky barrier (Left - before contact, Right – after contact). Notice that the barrier height is the difference between the energies of the Fermi level in the metal and the conduction band in the semiconductor.

The figure above shows a metal and a semiconductor with work functions φ_m and φ_s respectively, both before and after contact. When they are joined, the Fermi levels line up, and the same band-bending energy barrier and depletion region in the semiconductor are created as in a p-n junction.[3] This type of contact is known as *depletion*, and although the desirable contact type is *accumulation*, for doped silicon the type of contact formed is generally *depletion*.

The Schottky barrier is generally unavoidable in the formation of metal-semiconductor junctions. The way to eliminate this behavior, then, is not to eliminate the barrier, but to break it down. The barrier *height* is independent of the doping concentration in the silicon, but the barrier *width* does depend on the doping concentration. The barrier width decreases with increasing concentration of doping to the point that with high enough doping, quantum-tunneling effects begin to become pronounced and break down the barrier.[4] Electron flow in this way is called *field emission*.

The formation of NiSi proceeds by nickel flowing into silicon and forming the compound. As NiSi is formed, the dopants in the used portions of silicon are pushed back in a sort of snowplowing effect. Thus, the doping concentration at the metal-semiconductor interface after the completion of NiSi formation is very high, satisfying the requirement for the breaking down of the Schottky barrier, allowing low-resistance, ohmic contacts.

III. EXPERIMENTAL DETAILS – PART 1

Samples were created from four different silicon substrates, with varying doping concentrations. Metal pads were patterned, using photolithography and a liftoff procedure, with composition described in the figure below.

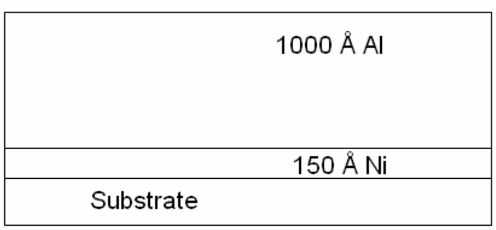

Figure 2 – Diagram describing sample structures - a thin nickel layer for silicide formation is followed by a thicker layer of aluminum, for electrical contact

The contact resistance was then measured, using a version of the Transfer Length or Transmission Line Method (TLM). TLM relies on resistance measurements between a series of pads with varying spacing.

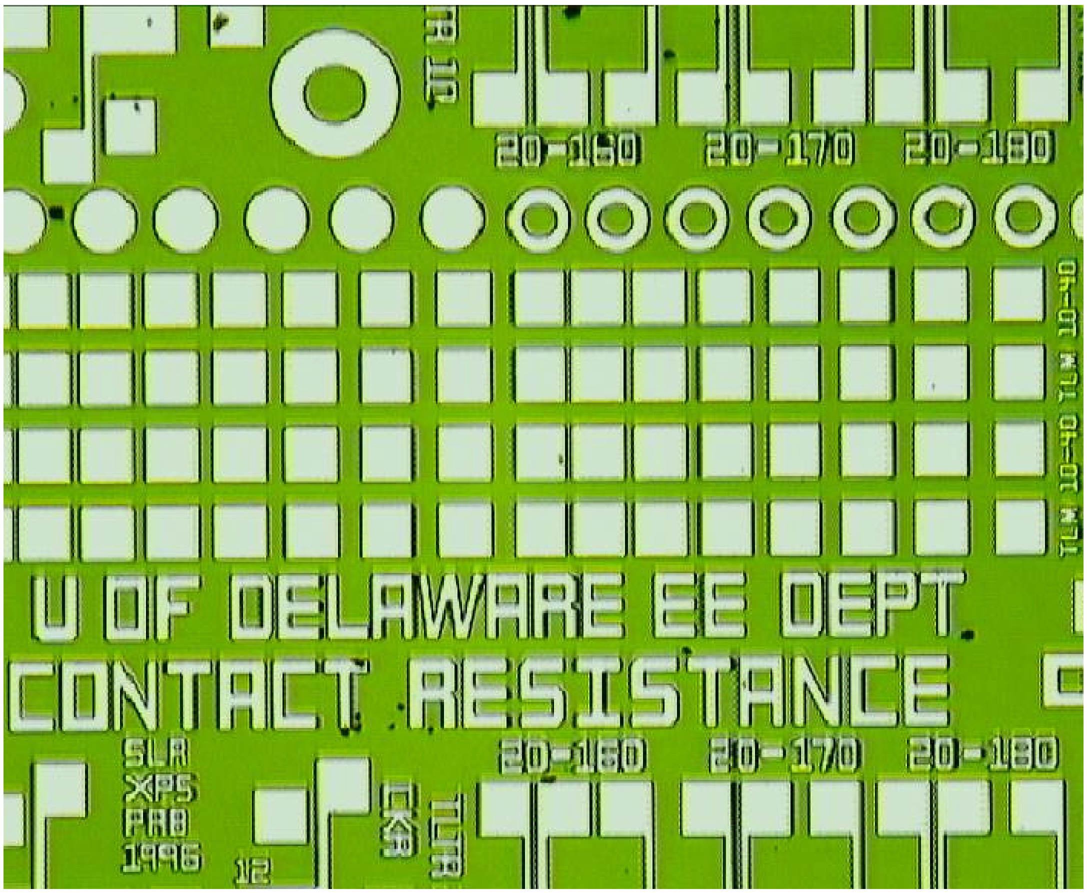

Figure 3 – Picture taken using a microscope, showing the TLM structures, with varying pad spacings. Each pad is 80 μm in each direction.

The resistance between any two pads, then, is considered to be

$$R_T = 2R_M + 2R_C + R_S \tag{1}$$

where R_T is the total resistance, R_M is the resistance of the metal pad, R_C is the contact resistance, and R_S is the resistance of the portion through the semiconductor. Assuming the resistance of the metal pad to be essentially zero, this reduces to

$$R_T = 2R_C + R_S \,. \tag{2}$$

Now, if we assume that the contribution from R_S is linearly dependent based on the distance between two pads, which is only a fair assumption in this case since the pads were not placed upon a mesa and the charge is not restricted to flowing in straight lines between pads, then at a pad spacing of zero, $R_S = 0$. This assumption is valid since a very accurate measure of contact resistance is not necessary for the purposes of this study. The y-intercept of a plot of R_T vs. pad separation, then, is approximately equal to $2R_C$, according to (2). Thus,

$$R_C = y_0 / 2 \tag{3}$$

describes the contact resistance. This description is sufficient for observing a reduction in contact resistance with silicide formation, but in order to allow comparison, another quantity, the specific contact resistivity ρ_c, must be calculated. The specific contact resistivity is a true measure of the quality of the contact, removing the dependence on pad size of the simple contact resistance. A derivation of its calculation is beyond the scope of this paper.

Four probes were needed to measure the resistance between any two pads accurately, two to provide a current between the pads, and two to measure the voltage between them. Since essentially no current could flow between the voltage monitoring probes due to high internal resistance, their measured voltage was only the difference between the two pads, independent of other factors like the resistance due to the probe contacts with the metal surface themselves.

Finally, a 60 second, 430° C rapid thermal anneal will be used to form NiSi, and the contact resistance will be measured both before and after this anneal for comparison.

IV. RESULTS – PART 1

Graphs of resistance vs. spacing were created for four different substrates of varying doping concentration, and these measurements were performed twice. A typical graph of Resistance vs. Pad Spacing looked like the one below.

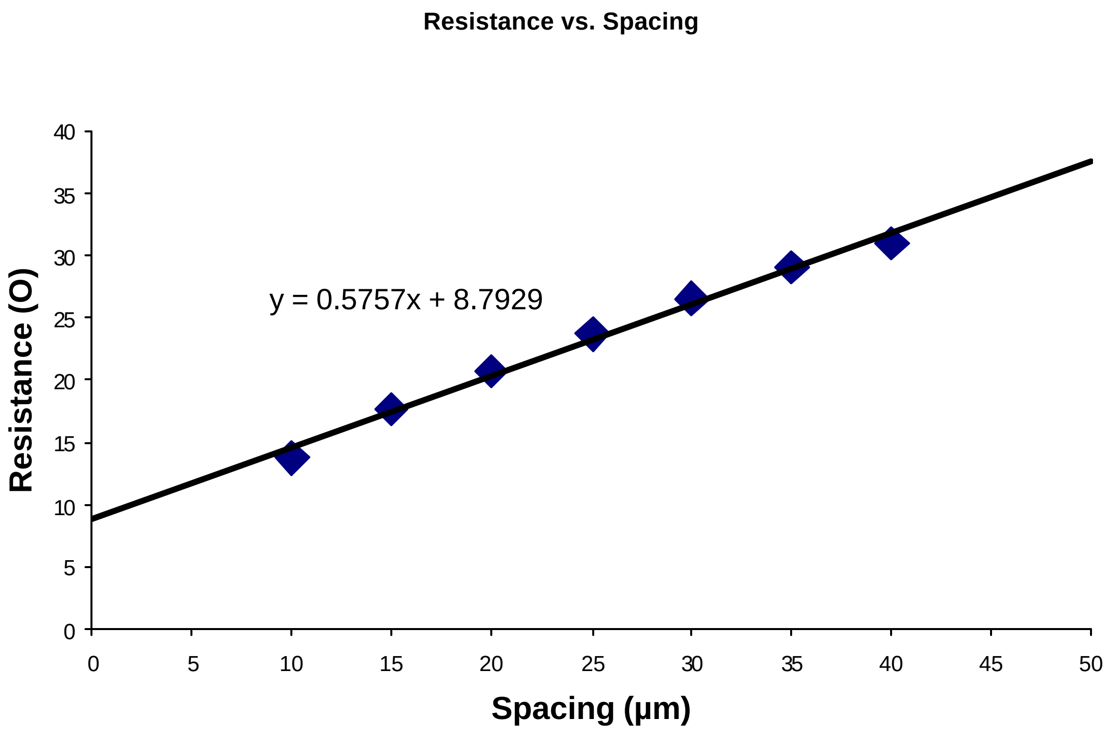

Figure 4 – A typical graph of Resistance vs. Spacing. Note that the y-intercept of the graph is equal to the contact resistance. This graph is for sample 90832.2

A similar plot was created for each of the samples both before and after the anneal at 430° C for 60 seconds. The figure below describes the effects of silicide formation.

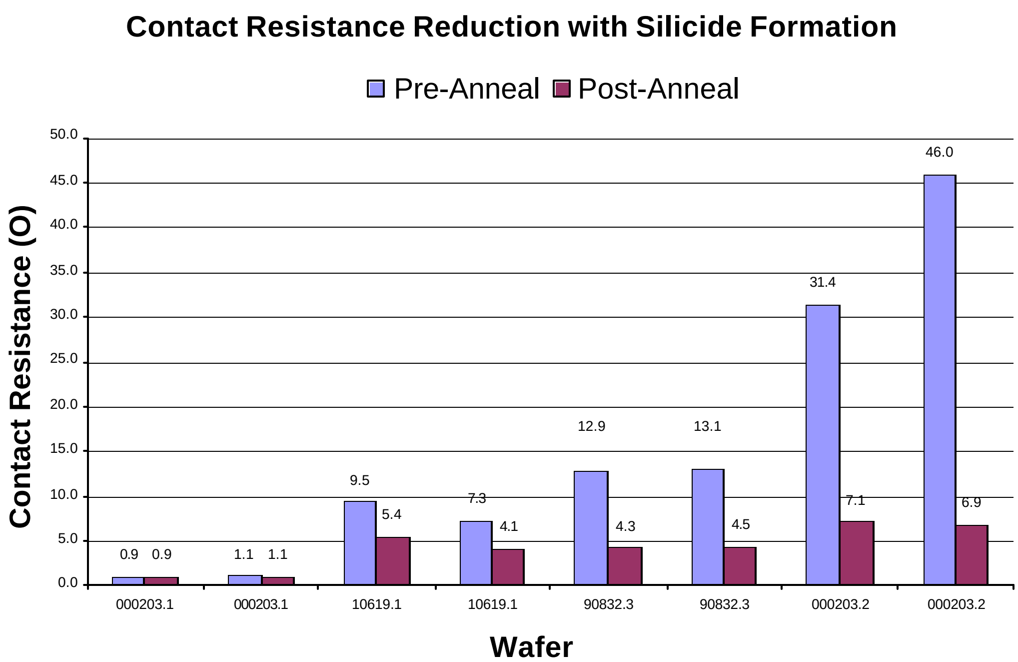

Figure 5 – Shows the reduction in contact resistance with annealing. Notice that there are two measurements for each wafer, as the measurement was done with two different sets of samples.

This figure suggests that NiSi is indeed formed under these annealing conditions, with a benefit to the contact resistance. What it cannot illustrate, however, is that the contacts started with a slightly rectifying behavior, and that this changed to a totally ohmic behavior after the anneal.

The specific contact resistivity even after annealing was also found to be somewhat dependent on the initial doping concentration, as well, as shown by the table below.

Sample	Approximate doping concentration (cm^-2)	Specific Contact Resistivity (ohm cm^2) (Trial 1)	Specific Contact Resistivity (ohm cm^2) (Trial 2)
000203.1	1E+20	4.47E-06	4.42E-06
10619.1	1E+19	4.31E-05	1.46E-04
90832.3	1E+19	2.50E-05	2.42E-04
000203.2	1E+18	4.92E-05	6.83E-04

Figure 6 – Illustrates the dependence of specific contact resistivity after annealing with initital doping concentration

This was also expected, since included in the specific contact resistivity is the resistance due to the sharp gradient of doping concentration in the silicon near the metal interface.

V. EXPERIMENTAL DETAILS – PART 2

In the second part of this experiment, diodes were created upon a sample with a simple p-n junction 1000 angstroms below its surface. The back side of the wafers were coated with a metal contact, and on the top side were patterned simple circles for the diodes, and a mesa was etched in the silicon substrate. The figure below describes this.

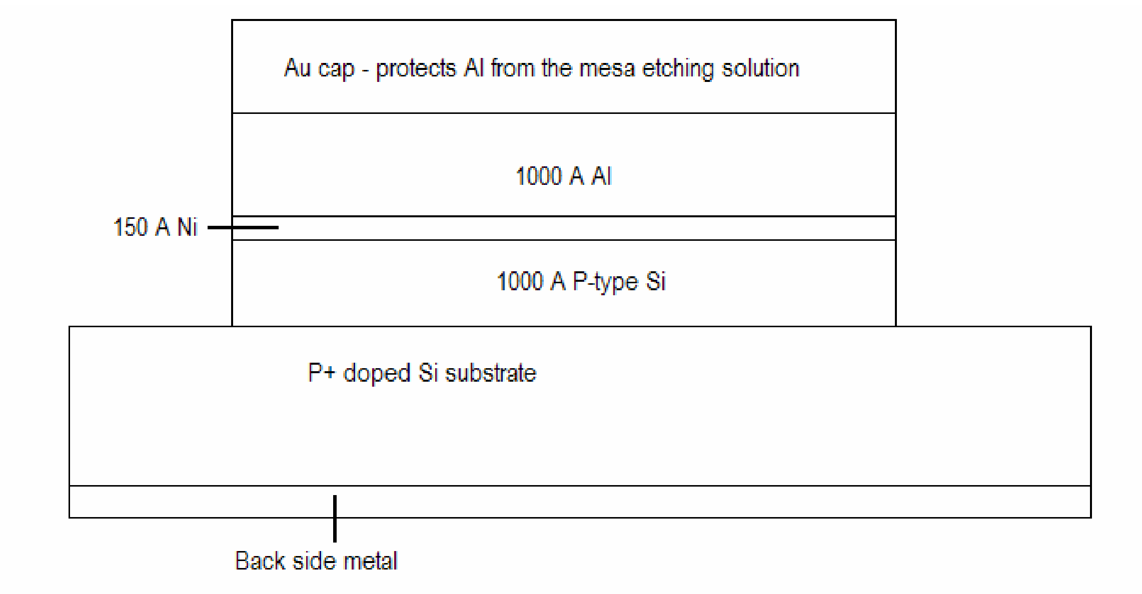

Figure 6 – Structure of simple diodes created for the testing of Al spiking

Also, two additional samples were created with the same structure as in Figure 6, except for a 300 angstrom barrier later between Ni and Al. The two samples used Cr and Mo as the material for this barrier layer, respectively. These two samples were unsuccessful, however, as will be discussed in the next section.

VI. RESULTS – PART 2

The diodes were first tested before any annealing, and functioned well. They were then exposed to a rapid thermal anneal of 450° C for 30 seconds, which is below a safety threshold for the stability that would be needed by the devices in order to withstand silicide formation, and the devices were found to be destroyed by this anneal. This effect was assumed to be a result of Al spiking.

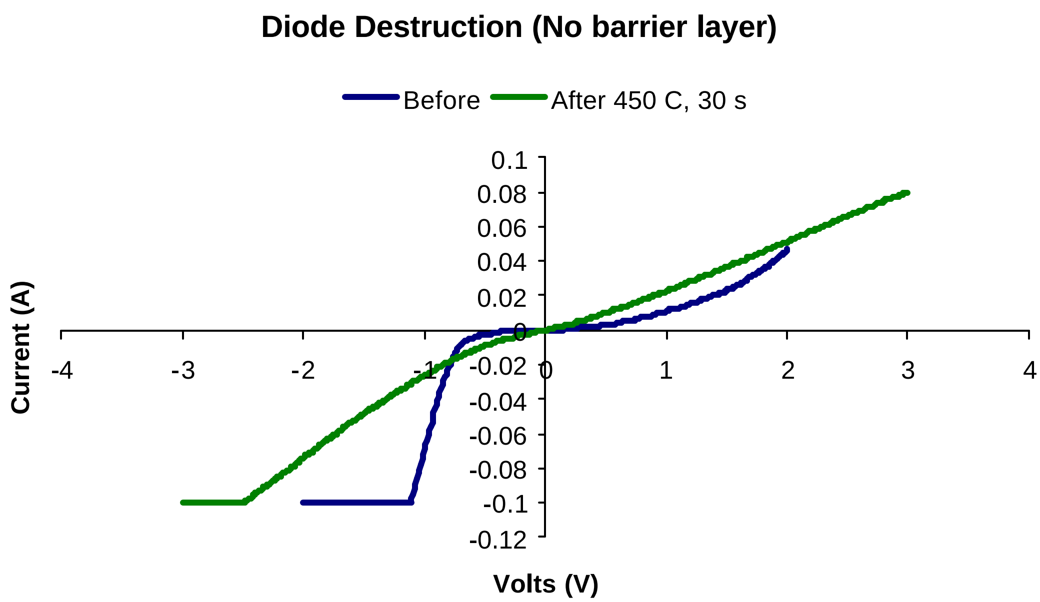

Figure 7 – Shows the destruction of the I-V characteristics of a diode after an anneal of similar characteristics to that required by NiSi formation

The samples with Cr and Mo barrier layers were unsuccessful. Those with a Cr barrier layer were destroyed by currents running through them as low as 40 mA, while previous devices had no problems with 100 mA. Those with a Mo barrier layer were overly baked in the metal deposition process, and destroyed during the mesa etch.

Figure 8 – Destruction of samples with a Mo barrier layer during mesa etch

VII. DISCUSSION / CONCLUSION

Nickel mono-silicide formation was indeed observed, and a reduction in contact resistance was apparent. The specific contact resistivities calculated after annealing (seen in Figure 6) were still in the 10^{-5}, 10^{-6} Ω cm^2 range, however, and increasing industry standards are requiring 10^{-7} for the contacts of the future. This suggests that future work is needed, either with NiSi or with another silicide-forming metal.

As can be seen in Figure 5, for sample 000203.1 the doping concentration wash high enough to begin with, almost to the point of δ-doping, that no real reduction in contact resistance was observed. This suggests that either 10^{-6} reflects some limit of the quality of contact with NiSi, or more precautions and cleaning measures need to be exercised in the production of the samples.

Additionally, the results of Part 2 suggest that great care needs to be taken to control Al spiking during the silicidation process, or else a very real threat of aluminum spiking down to the active region and shorting out devices exists. It appears that Al spiking is even more severe of a problem than was expected.

For the samples created with Cr and Mo barrier layers, likely a good first step for further research would be to simply remake the samples using extreme care, especially during the metal deposition and liftoff processes. If the same results are observed, we may begin to attribute the faults to such things as unforeseen reactions, but until then we do not have enough evidence to be sure that their production was not merely faulty. Certainly more work must be done to determine whether there was some inherent flaw with using these metals or not, and if so to continue looking for suitable barrier layers.

Acknowledgement

The authors would like to thank the Physics department for hosting the REU program, and the National Science Foundation for providing its funding. Special thanks also to Prof. Paul Berger and Ronghua Yu, for all of their help and input.

---

[1] Z. Shi et al, *Journal of Electronic Materials*, **32**, 185, (2003).
[2] Morimito et al, *IEEE Transactions on Electron Devices*, **42**, 917, (1995).
[3] P. Bhattacharya, *Semiconductor Optoelectronic Devices*, Prentice Hall Inc., Upper Saddle River, NJ, (1997).
[4] D. Schroder, *Semiconductor Material & Device Characterization*, John Wiley and Sons Inc. (1990).