Optical Constants of Ni$_{1-x}$Pt$_x$ and Ni$_{1-x}$Pt$_x$Si for Inline Metrology of Ohmic Contacts

Lina S. Abdallah,* Stefan Zollner, New Mexico State University, Las Cruces, NM
Christian Lavoie, Ahmet Ozcan, IBM, NY
Mark Raymond, GLOBALFOUNDRIES, 255 Fuller Rd., Albany, NY
* Now at Intel Corporation, 2501 NW 229th Ave, Hillsboro, OR

Variable Angle Spectroscopic Ellipsometry (VASE)
Graduate Students:
Lina Abdallah, Travis Willett-Gies, Nalin Fernando, Dennis Trujillo, Tarek Tawalbeh (Theory)

Undergraduate Students:
Cesar Rodriguez, Nathan Nunley, Khadijih Mitchell, Cayla Nelson, Laura Pineda, Eric DeLong, Luis Barrera, Chris Zollner (Cornell), Amber Medina, Maria Spies, Ayana Ghosh (Michigan-Flint)

Collaborators:
Igal Brener (CINT), Neha Singh, Harland Tompkins (J.A. Woollam Co.), S.G. Choi (NREL)

Samples: Demkov (UT Austin), Alpay (UConn), MTI (LAO), SurfaceNet (NIO), IBM, Ohio State

Flat & uniform films, at least 5 by 5 mm², low surface roughness, films on single-side polished substrate

Email: zollner@nmsu.edu

http://ellipsometry.nmsu.edu
Units of Optical Constants

• Wavelength $\lambda$ and photon energy $E$
  
  Wavelength: Specified in nm, $\mu$m, or Å
  Photon energy: Specified in eV
  $E=\hbar\omega=hc/\lambda$
  (633 nm equals 1.96 eV)

• Dielectric function, refractive index, and conductivity
  
  Complex dielectric function: $\varepsilon=\varepsilon_1+i\varepsilon_2$
  Complex refractive index: $n=N+ik$
  Optical conductivity: $\sigma=\sigma_1+i\sigma_2=\frac{-i\varepsilon_0 E(\varepsilon-1)}{\hbar}$

• For a metal, $n$ and $e$ diverge in the infrared due to the Drude response of free carriers. This divergence is avoided by the optical conductivity.
Spectroscopic Ellipsometry

Spectral range: 125 nm – 40 μm

\[
\rho = \frac{R_p}{R_s} = \frac{E_{rp}}{E_{ip}} \cdot \frac{E_{is}}{E_{rs}} = \tan \Psi \ e^{i\Delta}
\]

\[
\langle \tilde{n} \rangle^2 = \sin^2 \phi \left[ 1 + \tan^2 \phi \cdot \left( \frac{1 - \rho}{1 + \rho} \right)^2 \right]
\]

\[
\tilde{n} = n + ik
\]

\[
\tilde{\varepsilon} = \varepsilon_1 + i \varepsilon_2
\]

\[
\varepsilon_1 = n^2 - k^2 \quad \varepsilon_2 = 2 nk
\]

Optical conductivity

\[
\sigma_1 = E \varepsilon_0 \varepsilon_2
\]

\[
-\sigma_2 = (1 - \varepsilon_1)E \varepsilon_0
\]
Drude Model for Optical Constants of Metals

Dielectric function and optical conductivity

\[ \sigma_1: \text{Conductivity, absorption} \]
\[ \sigma_2: \text{Phase shift, dispersion} \]

\[ \sigma_0 = \frac{ne^2\tau}{m} = \frac{\varepsilon_0 E_p^2}{\hbar \Gamma} \]

\[ \sigma_2 \text{ has maximum at } E=\Gamma \]
\[ \sigma_1 \text{ and } \sigma_2 \text{ cross at } E=\Gamma, \text{ value is } \sigma_0/2 \]
Drude-Lorentz Model for Optical Constants of Metals

High reflection Coefficient

Outermost electrons shared by all the surrounding atoms

No band gap: almost any frequency of light can be absorbed.

For metal films $k \neq 0$, $\varepsilon$ is complex, decomposed into two components

$$\varepsilon = \varepsilon_{FCA} + \varepsilon_{bound}$$

Free carriers (Drude)  Bound carriers (Lorentz)
Ellipsometry Data Analysis

Experimental Data

- Well known material (Si, SiO₂)
  - Tabulated data
- New material (NiPt, NiPtSi)
  - Set of oscillators
  - Solve numerically

Build a model

2 Layer 2 \( t_2 \)
1 Layer 1 \( t_1 \)
0 substrate \( \infty \)

Generated Data

Compare Exp. And Gen. data

NO

Match ??

YES

Change model parameters

New Mexico State University

Stefan Zollner, 04/14/2015, Dresden, Germany
Frontiers of Characterization and Metrology for Nanoelectronics
Motivation: Metrology of NiSi for Ohmic Contacts

MOSFET: metal–oxide–semiconductor field-effect transistor

- Low resistivity
- Low formation temperature
- Low Si consumption

32 nm SOI CMOS (Greene et al.)
industrial self-aligned silicide process
Ni$_{1-x}$Pt$_x$ alloy samples and experimental details

- Films were deposited using **Physical Vapor Deposition (PVD)**.
- Different Pt concentrations (0%, 10%, 15%, 20%, 25%)
- with/without annealing (500°C for 30 s)
- Low surface roughness.
- 300 mm wafers.
- Rough backside.

- Room temperature measurements.
- **Fourteen angles of incidence (20° to 80°, steps of 5°)**
- Broad photon energy range (0.6 to 6.6 eV), 20 meV steps, 300 data points per angle. **2 nm resolution (1 mm slits)**
- Each measurement lasts **24 hours**.
Optical constants of Ni and Ni$_{1-x}$Pt$_x$ alloys

- **Optical Conductivity**
  
  \[ \sigma_1 = E\varepsilon_0\varepsilon_2 \]
  
  \[ -\sigma_2 = (1 - \varepsilon_1)E\varepsilon_0 \]

- **Dielectric Function**
  
  \[ \varepsilon_2 \] Describes absorption

---

Stefan Zollner, 04/14/2015, Dresden, Germany
Frontiers of Characterization and Metrology for Nanoelectronics

New Mexico State University

http://ellipsometry.nmsu.edu
Optical constants of Ni and Ni$_{1-x}$Pt$_x$ alloys

Pt 5d bands are broader than Ni 3d bands.

Thus, peaks in Ni$_{1-x}$Pt$_x$ alloys are broader than in pure Ni.

Stefan Zollner, 04/14/2015, Dresden, Germany
Frontiers of Characterization and Metrology for Nanoelectronics
Water absorption metals could be a problem

- Ni-Pt alloy on thick thermal oxide.
- Keep in air for a year: 53 Å of water
- Heat in UHV for an hour: 7 Å of water

Must de-gas wafer before ellipsometry measurement to remove atmospheric molecular contamination (water, solvents, etc).
NiSi Formation

NiSi: Unstable at high temperatures

NiSi₂ formation
Agglomeration (thin films)

280 °C
NiSi₂
Metal rich silicides

350 °C
NiSi
Node rich silicide

750 °C
NiSi₂
Silicon rich silicide

Effects of additive elements on the phase formation and morphological stability of nickel monosilicide films

Microelectronic Engineering 83, 2042 (2006)
Ellipsometry of silicide films on Si

- Ni$_{1-x}$Pt$_x$ (0%, 10%, 20%, 30% Pt)
- Anneal 500°C for 30 s
- Thickness of resulting silicide $\approx 2 \times$ metal thickness
- SiO$_2$ is native oxide on NiSi.
- Three angles of incidence: 65° to 75°
- Vary thickness of silicide to minimize Si substrate artifacts in pseudo-dielectric function.

Stefan Zollner, 04/14/2015, Dresden, Germany
Frontiers of Characterization and Metrology for Nanoelectronics
Monosilicide:
Vary thickness of silicide to minimize Si substrate artifacts

Arwin & Aspnes 1984

E₁ of Si
Optical constants of Ni$_{1-x}$Pt$_x$Si

0% Pt
240 Å

10% Pt
230 Å

20% Pt
220 Å

30% Pt
200 Å

http://ellipsometry.nmsu.edu
Optical constants of $\text{Ni}_{1-x}\text{Pt}_x\text{Si}$

Broadening increases as Pt content gets larger.

| SiO$_2$ | Oscillator model $\text{Ni}_{1-x}\text{Pt}_x\text{Si}$ | Si |

Oscillator Model:
1 Drude (Free electrons + Intraband transitions)
5 Lorentz oscillators (Interband transitions)

http://ellipsometry.nmsu.edu

Stefan Zollner, 04/14/2015, Dresden, Germany
Frontiers of Characterization and Metrology for Nanoelectronics
Summary: Optical constants of $\text{Ni}_{1-x}\text{Pt}_x$ and $\text{Ni}_{1-x}\text{Pt}_x\text{Si}$

- Ellipsometry can measure metal and silicide film thicknesses. Some sensitivity to Pt content (broadening).
- Data posted at [http://ellipsometry.nmsu.edu](http://ellipsometry.nmsu.edu).
- Pt content broadens interband transitions in metal and silicides, because Pt-5d bands are broader than Ni-3d bands.
- NiPtSi optical conductivity exhibits metallic behavior due to the metallic content as well as interband transitions due to silicon-related electronic states.
- Free carrier absorption is stronger for unreacted metal than for silicide. However, interband transitions stronger for silicides.
- Interband transition peak gets broader with increasing Pt content in the silicide (can be explained in terms of NiPt DOS).
All data (real and imaginary parts of the dielectric function versus photon energy) are posted on our web page: http://ellipsometry.nmsu.edu.

We are available to measure flat films deposited by others using our high-accuracy Woollam VASE with autoretarder. Contact zollner@nmsu.edu.


L. Abdallah, T.M. Tawalbeh, I.V. Vasiliev, S. Zollner, C. Lavoie, A. Ozcan, and M. Raymond, *Optical conductivity of Ni$_{1-x}$Pt$_x$ alloys (0<x<0.25) from 0.76 to 6.6 eV*, AIP Advances **4**, 017102 (2014).
