Optical Properties of Sputtered Tantalum Nitride Films Determined by Spectroscopic Ellipsometry

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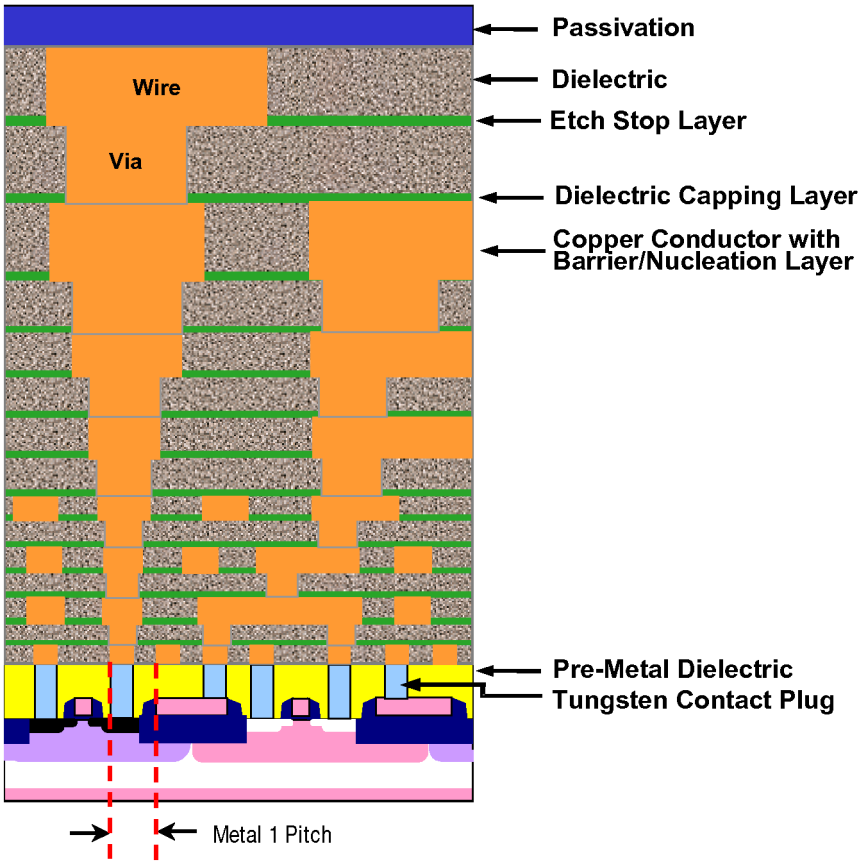
Motivation

Ta and TaN in Microelectronics Metallization

- Complex multilevel metallization systems
- Cu preferred conductor material for high-performance ULSI
- Diffusion barriers required:
  - TaN/Ta established material system
  - Thickness < 10nm (!)
- Fabrication:
  - Physical Vapor Deposition (e.g. long-throw sputtering and IPVD)
  - Atomic Layer Deposition (ultra-thin barriers)



(International Technology Roadmap for Semiconductors, http://public.itrs.net)

Experimental Details

Sample Preparation

- Reactive magnetron sputtering in Ar/N_2 plasma at room temperature
- TaN films with different stoichiometry:
  - Ta standard samples ($Ar:N_2$ flow = 4 : 1) ***[standard TaN]***
  - Ta rich samples ($Ar:N_2$ flow = 26 : 1) ***[modified TaN]***
- Samples:
  - Single thick films of Ta and TaN, 75nm to 380nm thick
  - Film stacks of TaN (standard, 20nm) / Ta (20nm) on Si and SiO_2

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Experimental Details

Sample Characterization

Structural and morphological aspects:

- SEM, TEM, AFM, XRD

Spectroscopic ellipsometry:

- SENTECH SE 850 spectroscopic ellipsometer
- Spectral range: 190 nm to 2.55 µm
- Lorentz-Drude models derived
- n,k and film thicknesses extracted

Structure and Morphology

Thick Films

Tantalum:

- β-Ta grown
- (002) oriented [consitent with earlier results [1]]

Tantalum Nitride:

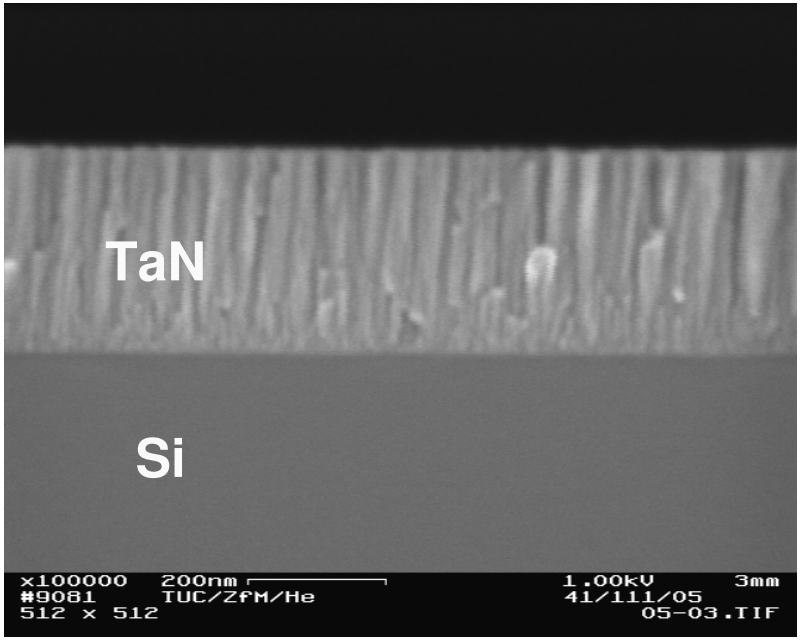
- Polycrystalline
- Strongly disordered (broad X-ray diffraction peaks)
- Small crystallites (lateral size: 24-36nm)

Standard:

- Columnar growth
- fcc TaN (TED)
- Stoichiometric

Modified:

- Ta_2N/Ta_4N mix



Cross-sectional SEM image of 290nm thick TaN film on Si.

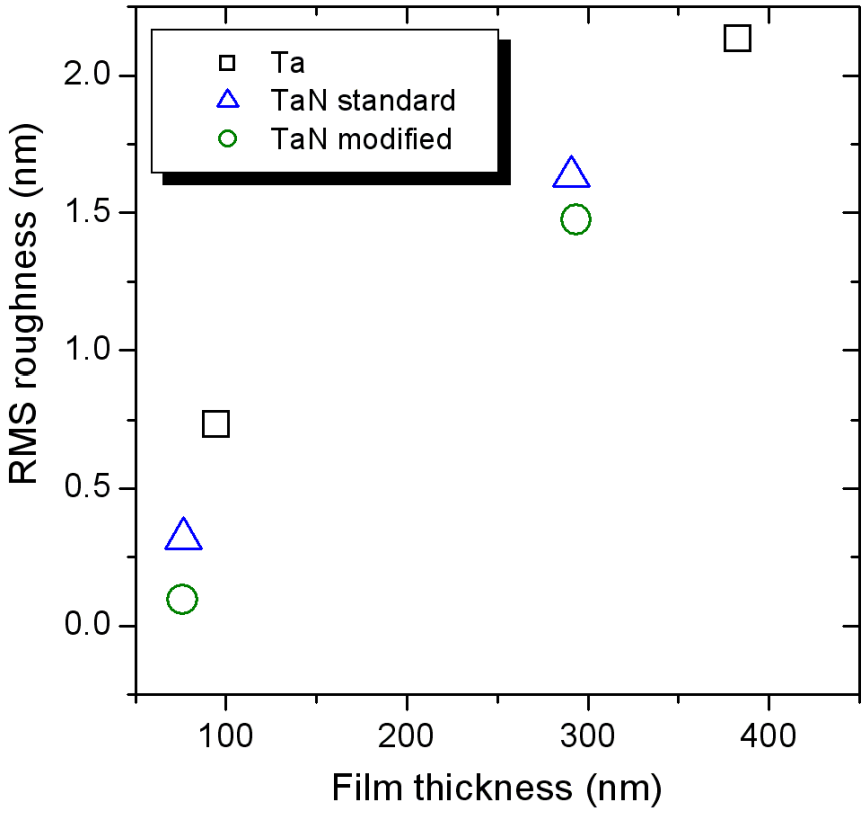
[1] J. Baumann, PhD Thesis, TU Chemnitz, 2003.

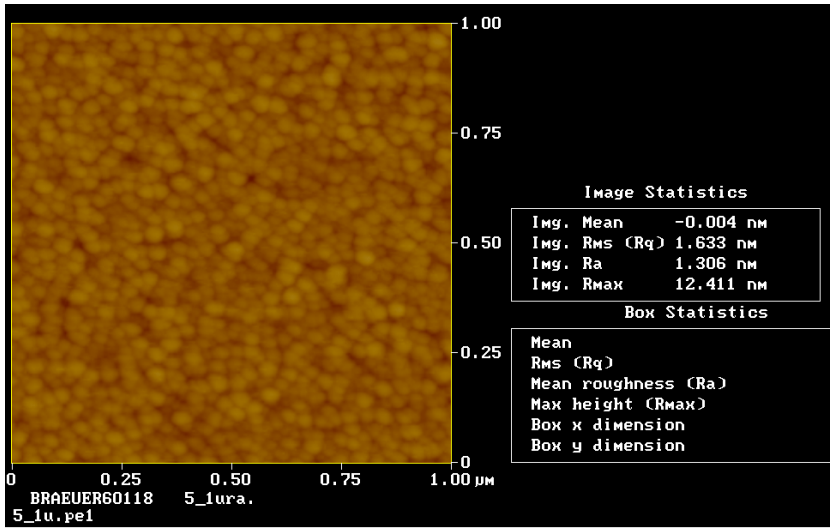
Structure and Morphology

Thick Films

Smooth films obtained:

- RMS roughness 0.1 to 2.1 nm



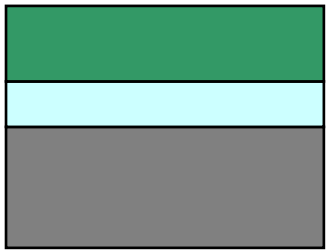


AFM analysis of 290nm thick TaN film.

Ellipsometry

TaN Films

- Starting model: Lorentz-Drude approach for TiN (3 oscillators)
- 75nm standard TaN film: optically transparent → film thickness determined



TaN 74.4nm (SEM: 76.4nm)

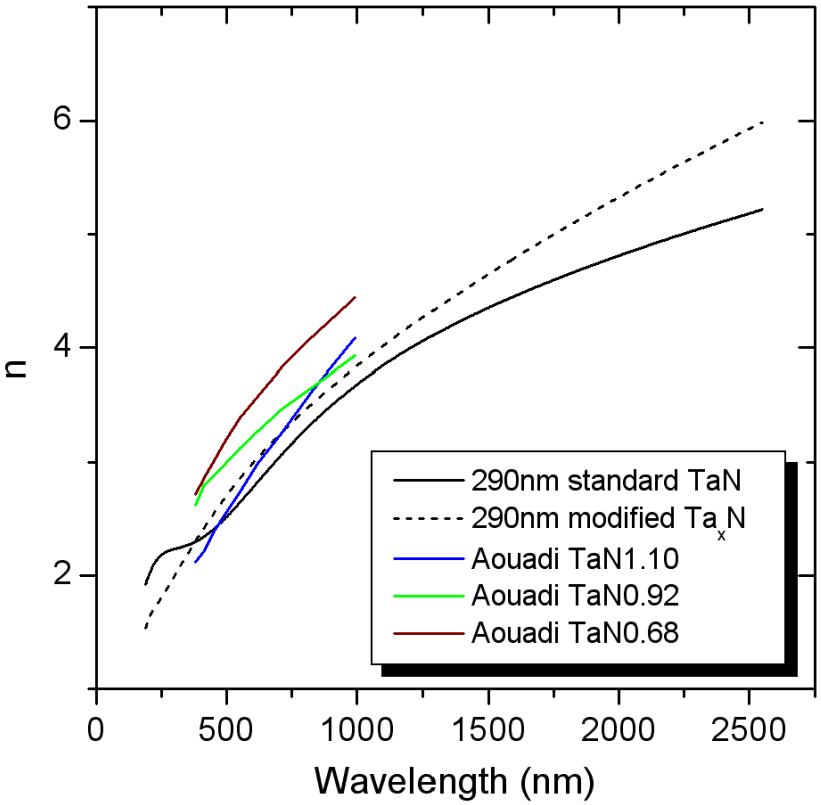
Native SiO_2 1.8nm

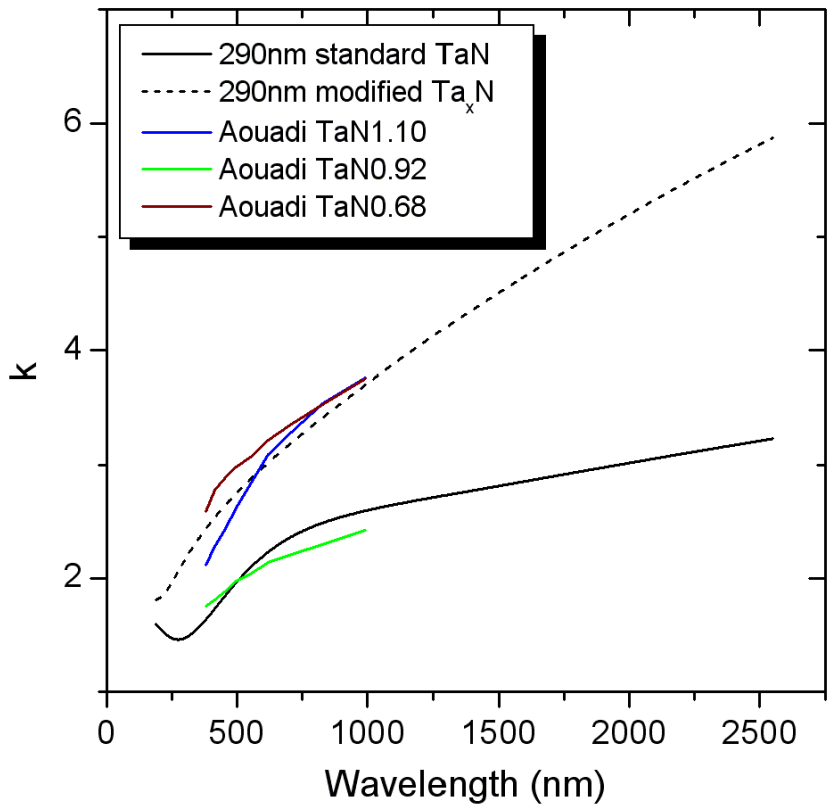
Si (substrate)

- Thicker films and all Ta-rich samples opaque

Ellipsometry

TaN Films



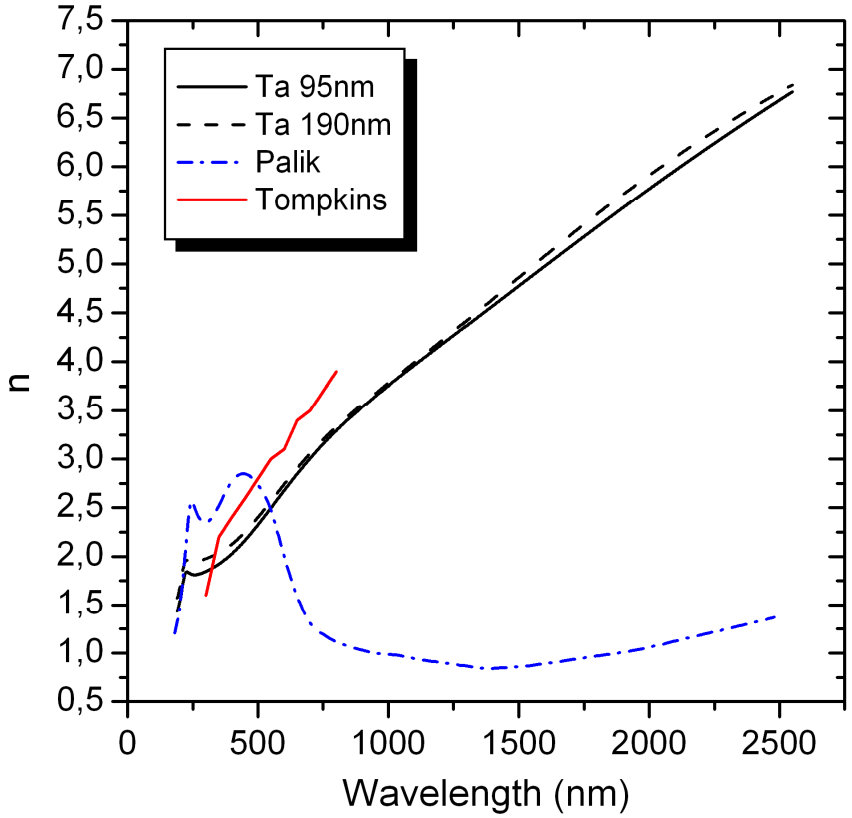


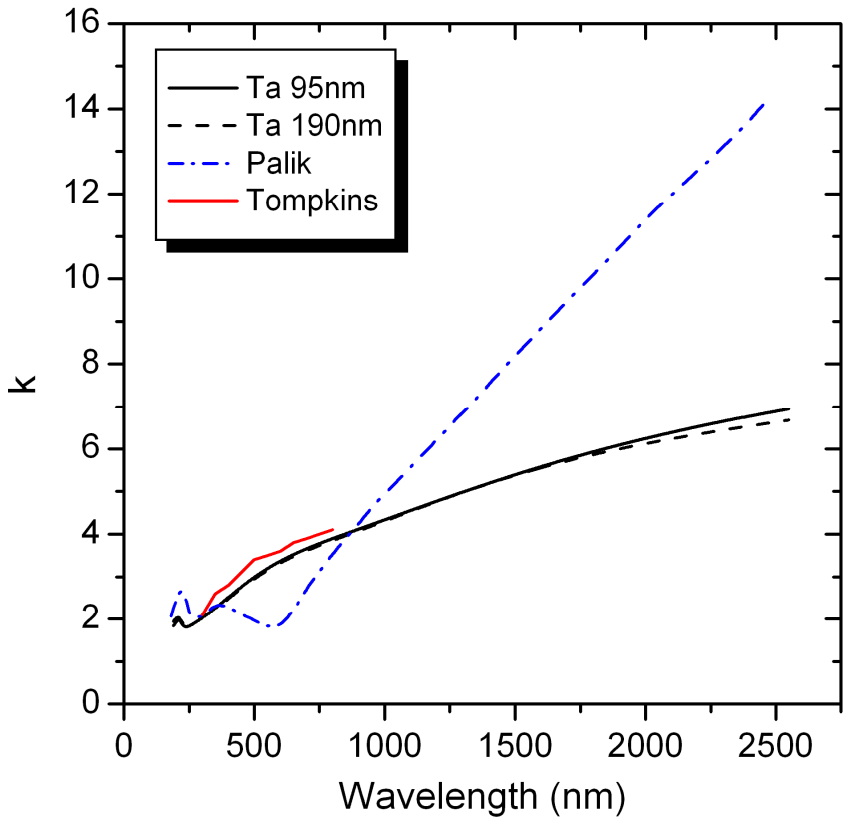
- Significant differences between TaN and Ta_2N/Ta_4N samples
- Values and curve shape close to literature data

  [S.M. Aouadi, M. Debessai, *J. Vac. Sci. Technol. A* **22** (5), 2004]

Ellipsometry

Ta Films





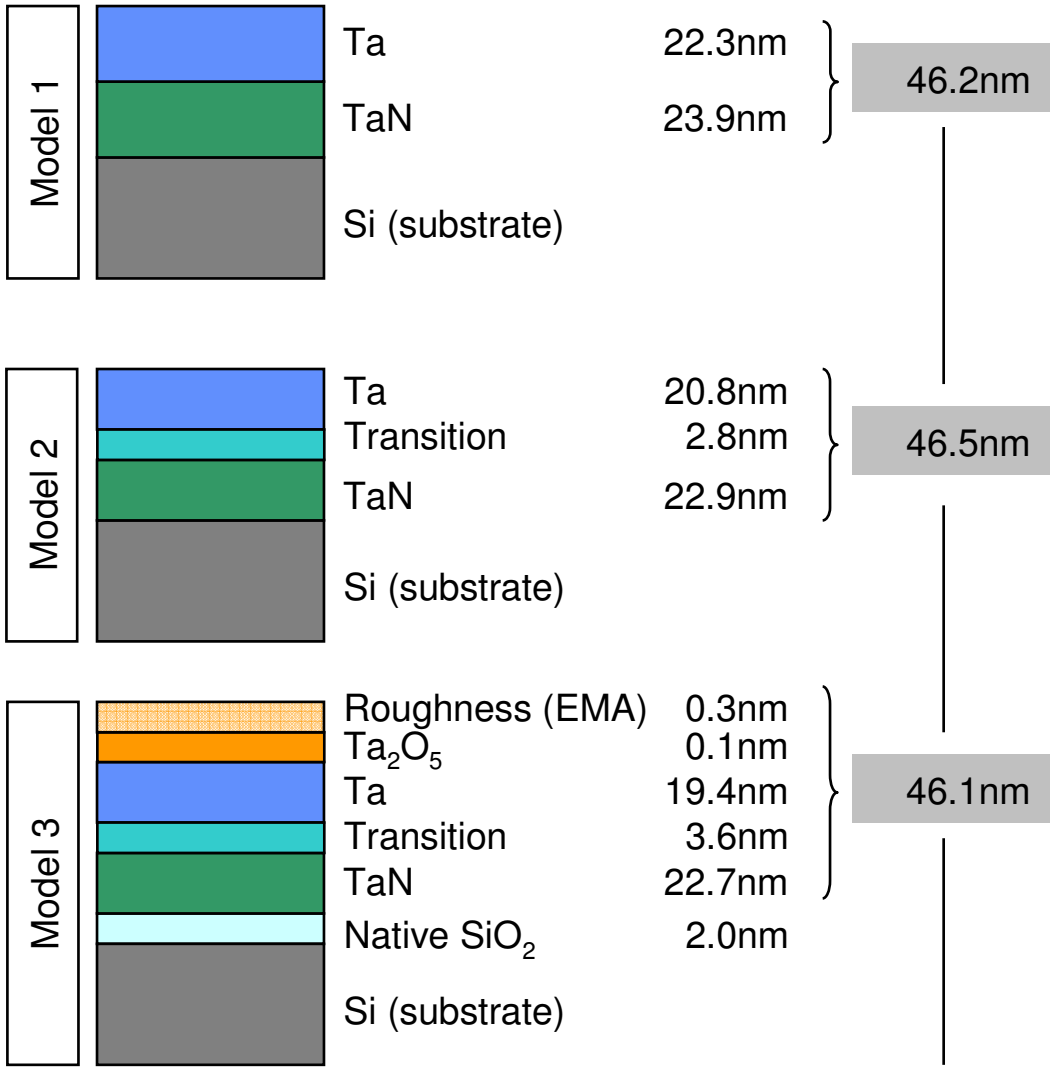
- Similar results for different film thicknesses (opaque samples)
- Consistent with literature data for sputtered 100nm films (“Tompkins”)
- Considerable differences to bulk data for α-Ta (“Palik”)

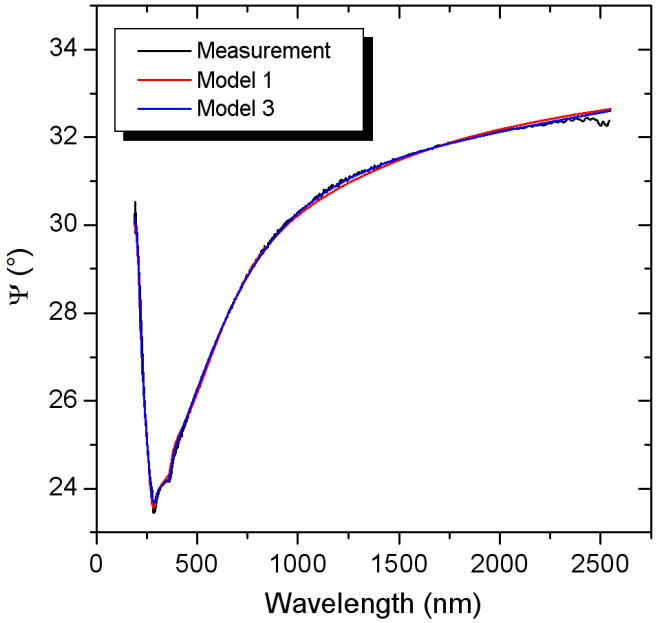
“Palik”: Handbook of Optical Constants of Solids II (ed. by E.D. Palik), Academic Press, 1998

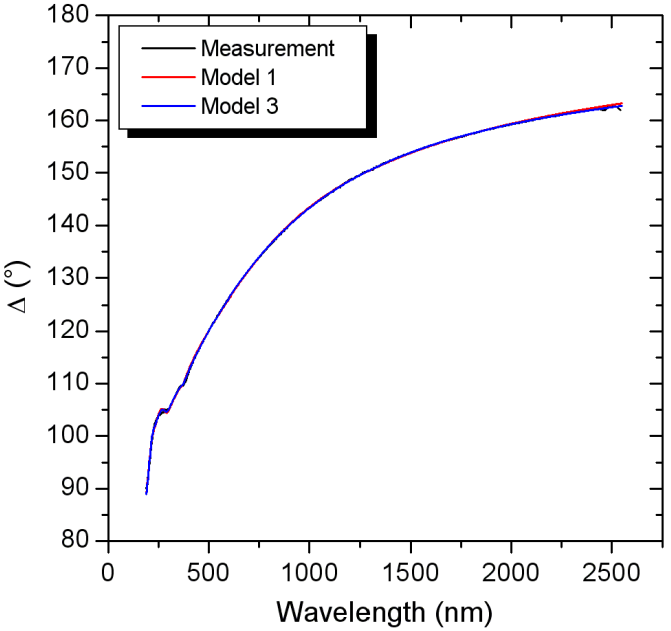
“Tompkins”: H.G. Tomkins, T. Zhu, E. Chen, *J. Vac. Sci. Technol. A* **16** (3), 1998

Ellipsometry

TaN (20nm) / Ta (20nm) on Si

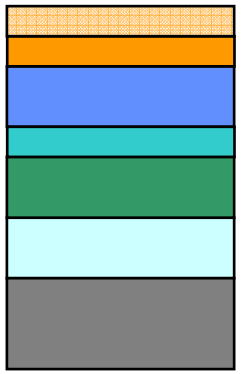






Ellipsometry

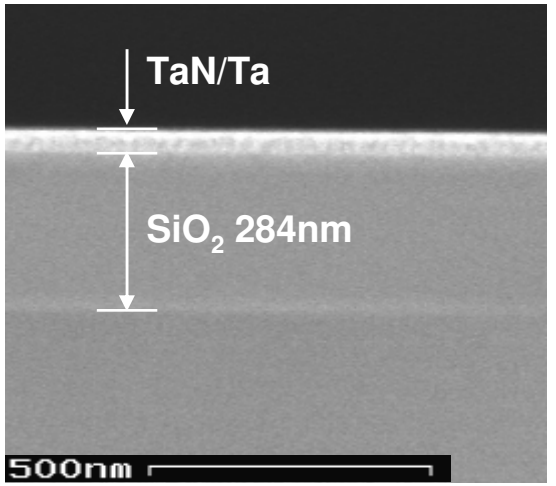
TaN (20nm) / Ta (20nm) on thermal SiO_2

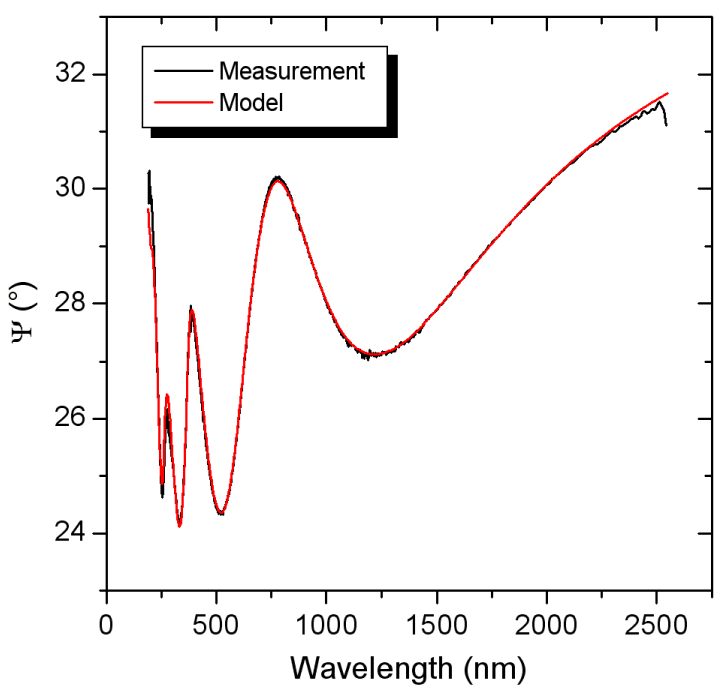


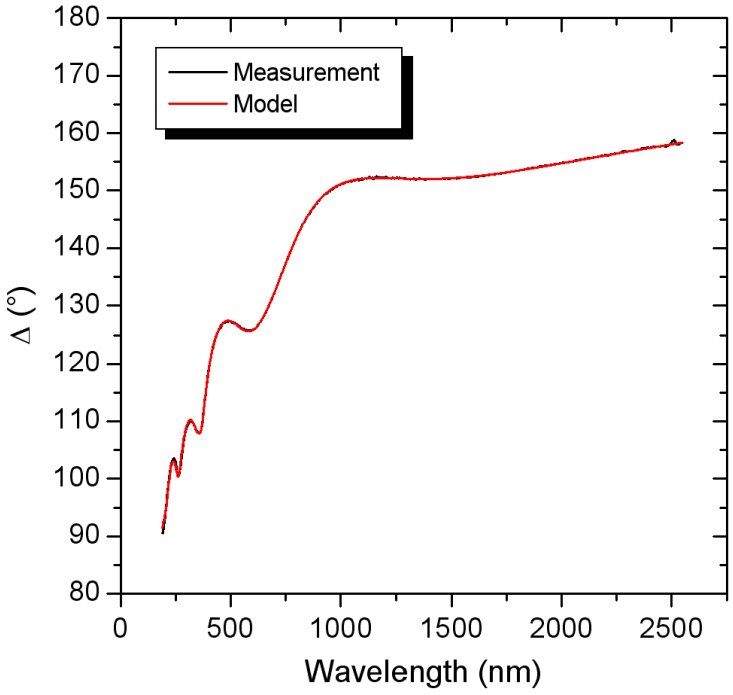
Roughness (EMA)	0.9nm
Ta_2O_5	1.3nm
Ta	17.3nm
Transition	1.8nm
TaN	20.4nm
Thermal SiO_2	295.9nm
Si (substrate)	

41.7nm

SEM (TaN+Ta): 43.5nm







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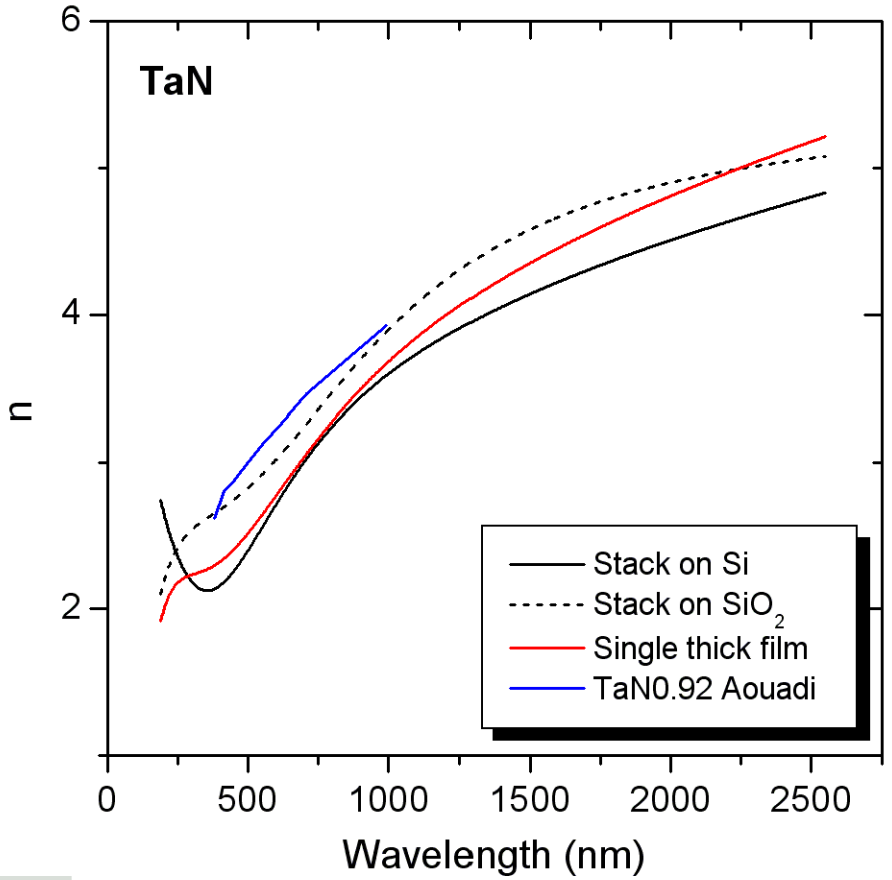
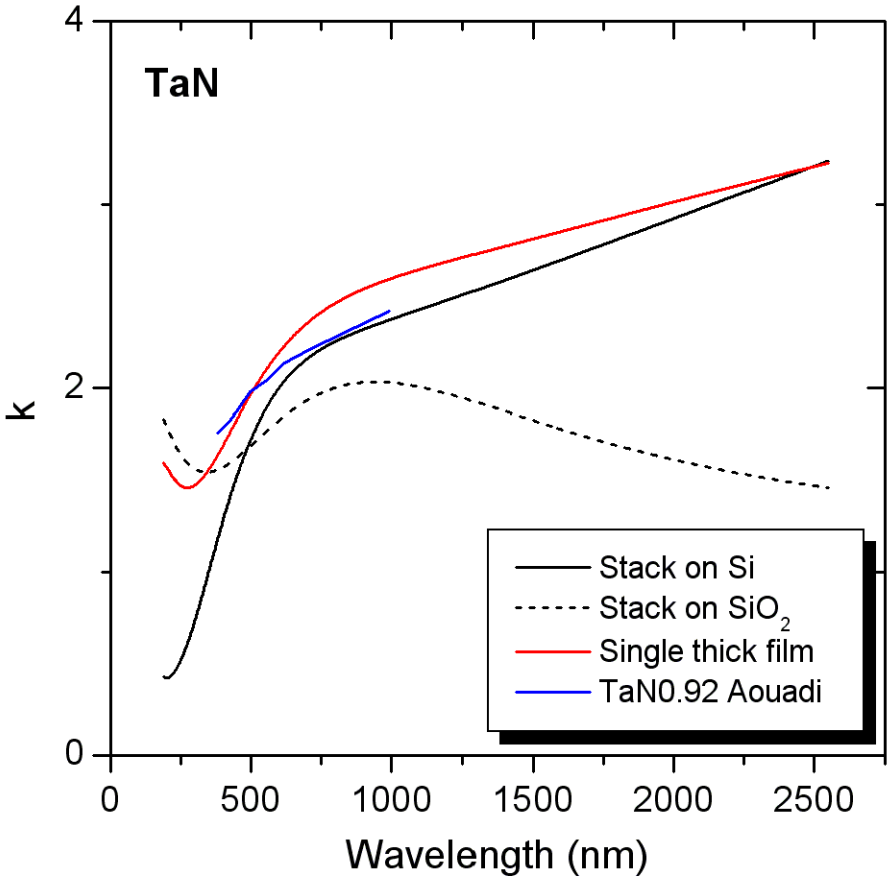
Discussion

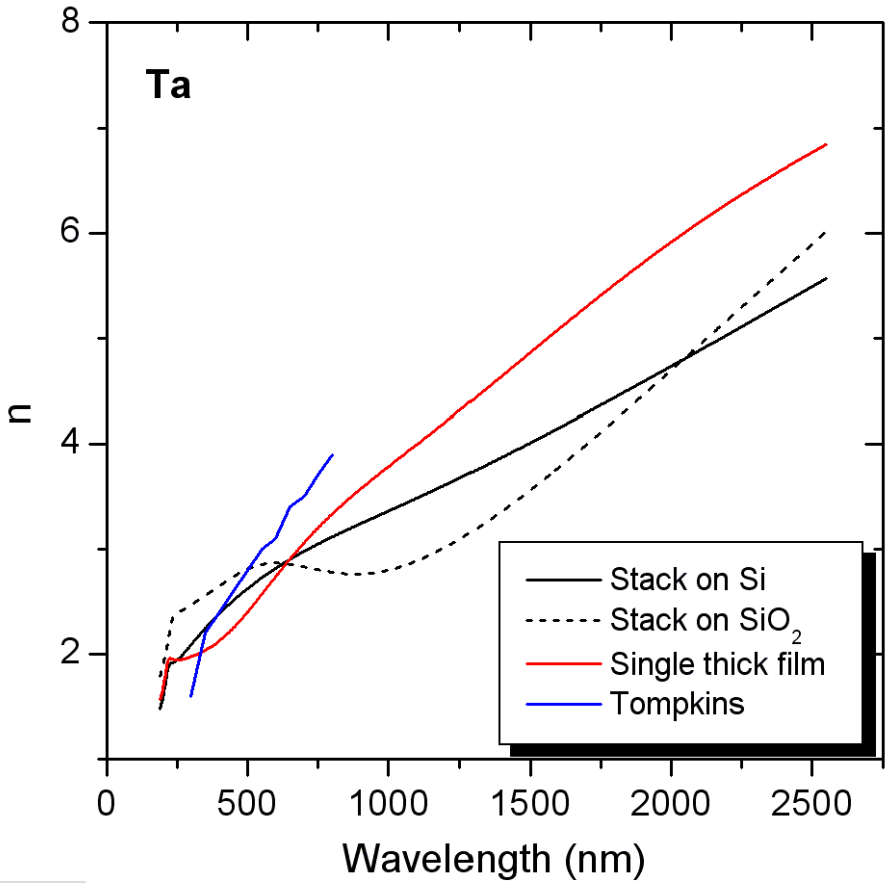
Comparison of Optical Property Data

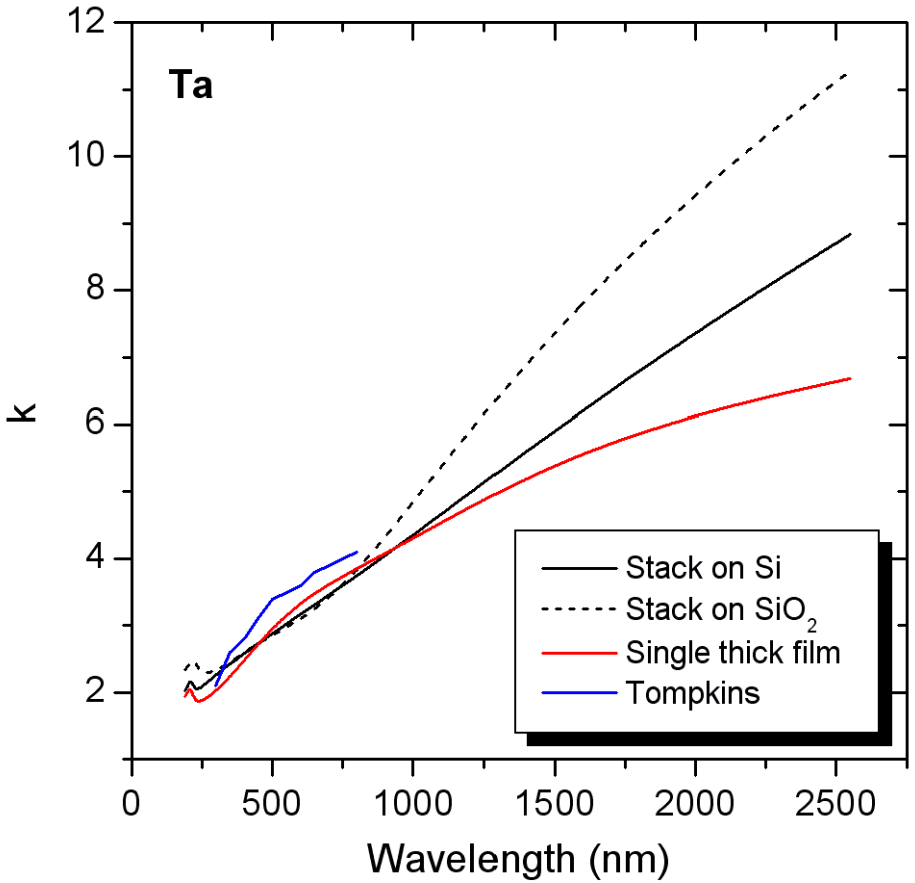




Discussion

Comparison of Optical Property Data





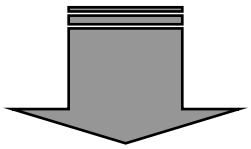
Discussion

Comparison of Optical Property Data

- Reasonable fits in cases with variable oscillator parameters
- Film stacks reproduced well
- Significant differences in optical properties depending on film thickness and substrate

→ Substrate influences TaN growth

→ TaN might then affect Ta growth (at least 3 Ta and 9 TaN phases known[1])



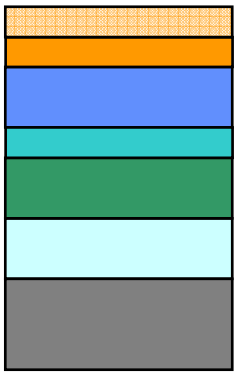
Real??

[1] J. Baumann, PhD Thesis, TU Chemnitz, 2003; and references cited therein

Ellipsometry

TaN (20nm) / Ta (20nm) on thermal SiO_2

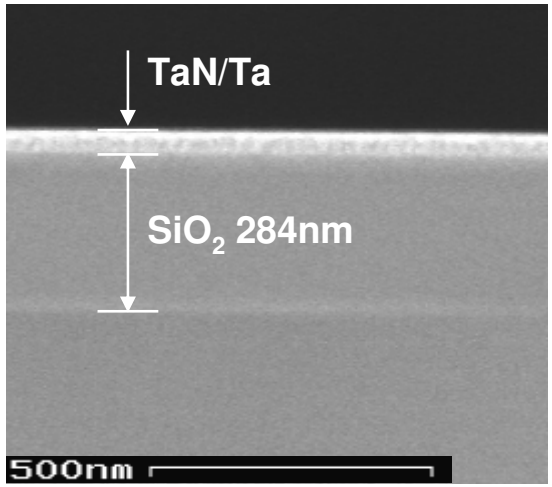
Modeling with constant oscillator parameters:

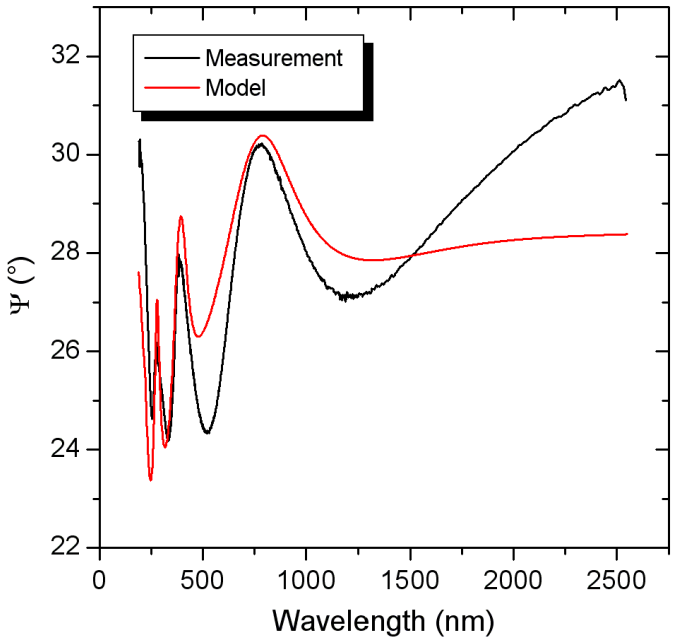


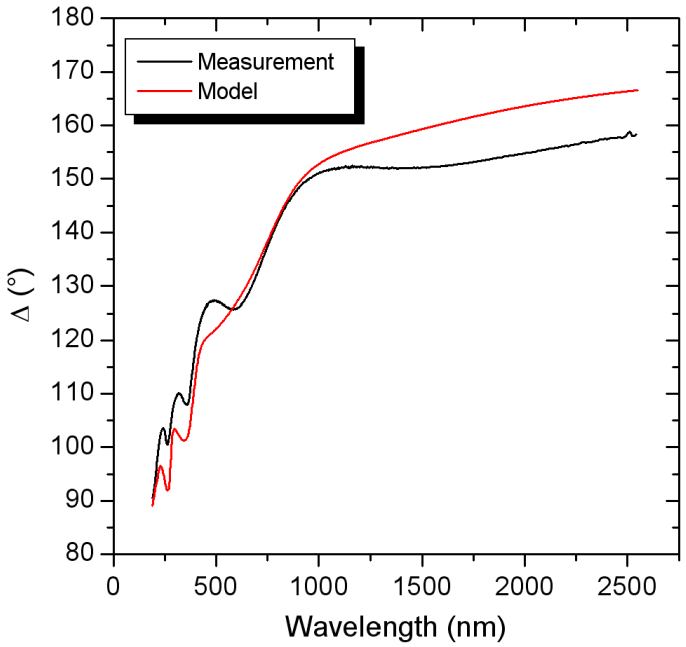
Roughness (EMA)	0.0nm
Ta_2O_5	0.0nm
Ta	31.1nm
Transition	0.0nm
TaN	5.0nm
Thermal SiO_2,	319.1nm
Si (substrate)	

36.1nm

SEM (TaN+Ta): 43.5nm







Bad fit!

Conclusions and Summary

- Ta and TaN films grown by reactive magnetron sputtering
- Optical properties determined by spectroscopic ellipsometry **(UV-VIS-NIR)**

Single thick films:

- Thickness of ~75nm TaN measured, thicker and Ta-rich films opaque
- Good agreement with **narrow-band** data for thin Ta and TaN films
- Optical properties of thin-film Ta considerably different from bulk material (α vs. β phase)

Film stacks 20nm TaN/20nm Ta:

- Good fits for TaN/Ta stacks on Si and SiO_2 obtained
- Thicknesses of TaN and Ta films correctly determined with free oscillator parameters
- Optical properties strongly dependent on substrate (→ growth mode, phase) and film thickness

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  TU Chemnitz, Solid Surfaces Analysis Group
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- **Jürgen Bräuer (AFM)**
  TU Chemnitz, Opto and Solid-State Electronics Group

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Further Details

Structure and Morphology

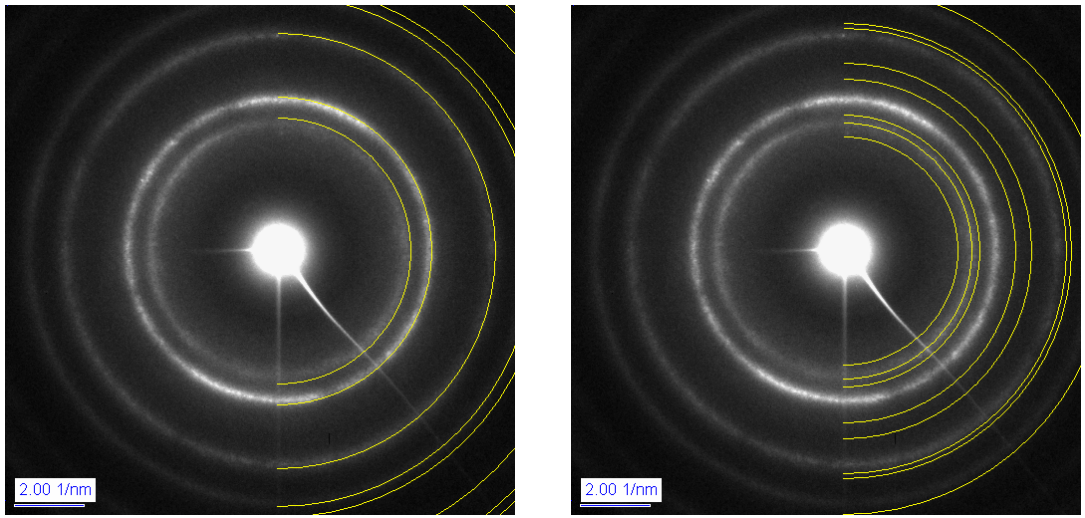
Thick Films

Standard TaN (N rich):

- Mixture of fcc and hexagonal TaN phases (XRD)
- fcc phase preferred (TED)

Modified Ta_xN_y (Ta rich):

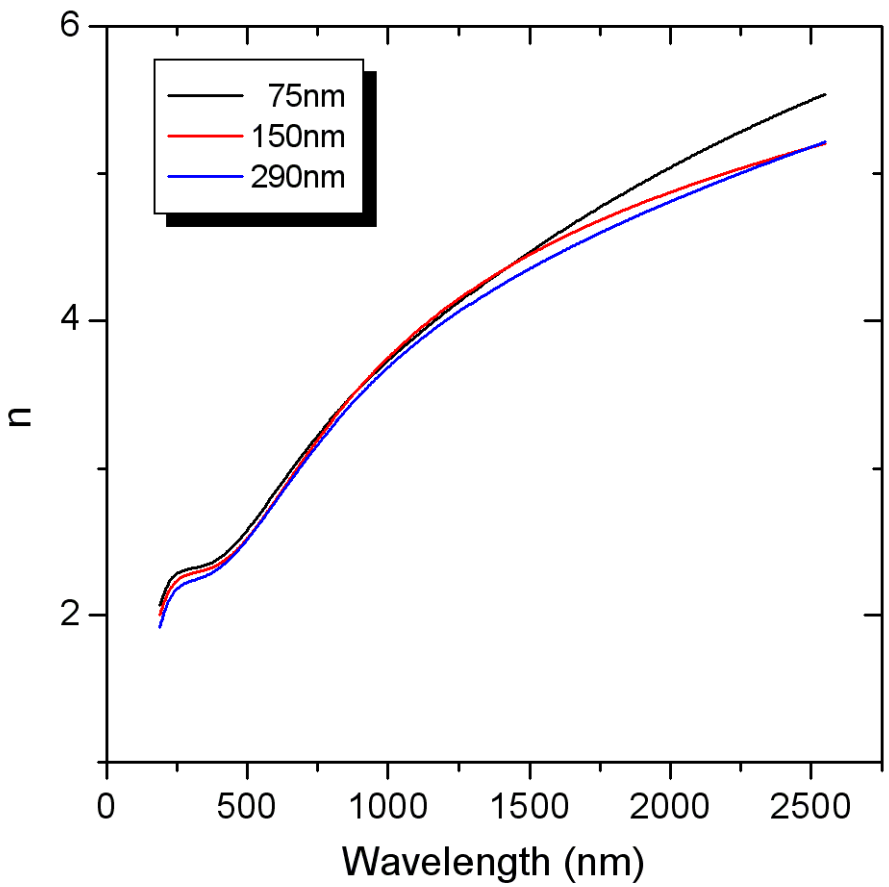
- Mixture of Ta_2N and Ta_4N stoichiometries (XRD)

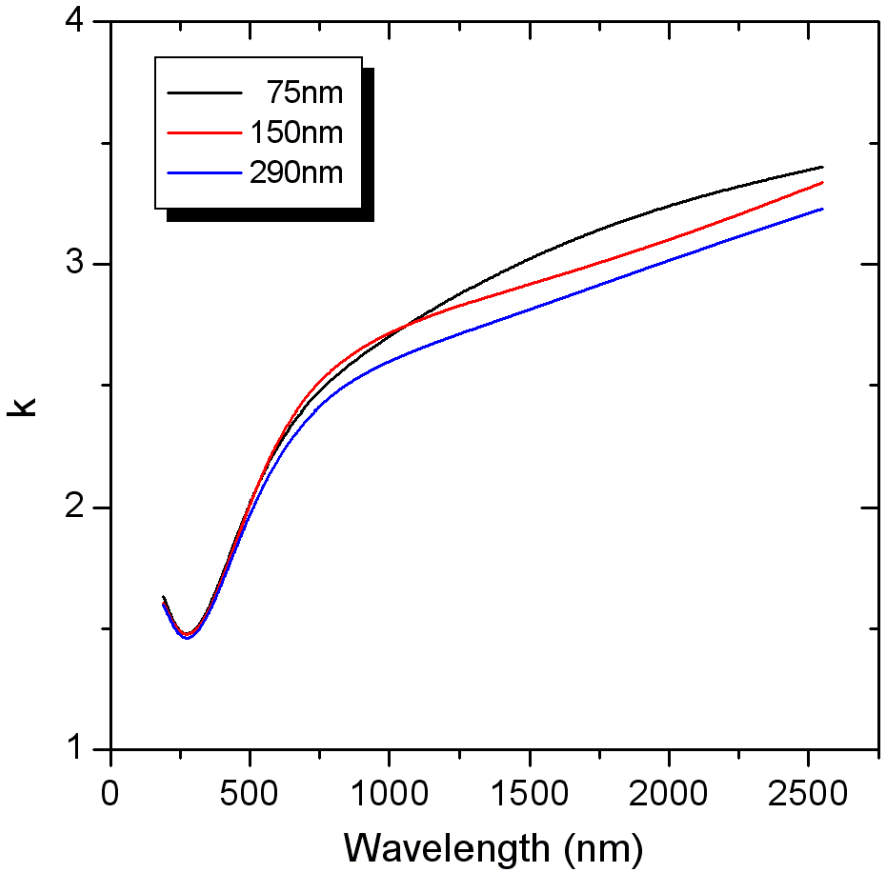


Electron diffraction patterns for standard TaN compared with theoretical patterns (yellow) for the fcc (left) and hexagonal phase (right).

Ellipsometry

TaN Films





Optical properties of standard TaN films from 75nm to 290nm thickness.