



Growth of TiO₂ thin films by high power impulse magnetron sputtering

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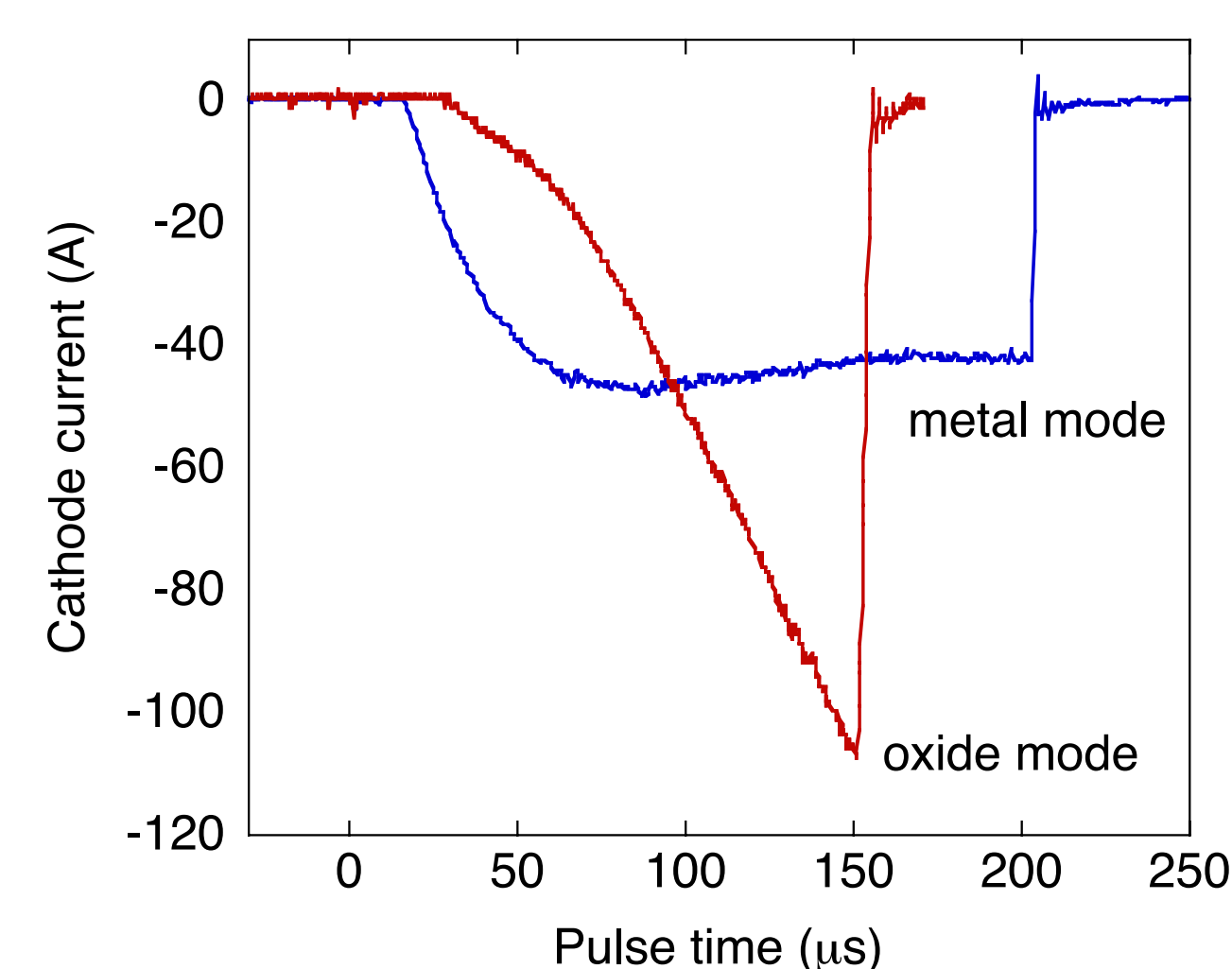
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Introduction

- High power impulse magnetron sputtering (HiPIMS) is an emerging ionized physical vapour deposition technique [1]
- By pulsing the sputtering target with high power ($\sim 1 \text{ kW/cm}^2$), short duration ($\sim 100 \text{ }\mu\text{s}$) pulses, a high ionization of the sputtered species is obtained, without significant target heating
- HiPIMS has been shown to have several advantages over conventional dc magnetron sputtering (dcMS) including increased film density, lower roughness, increased reactivity at low temperatures and better step coverage [2]
- The aim of this study is to compare thin TiO₂ films grown by HiPIMS and dcMS at various substrate temperatures
- TiO₂ finds application in a variety of electrical and optical devices due to its high refractive index and good thermal stability
- Structural properties are examined by grazing incidence X-ray diffraction (GIXRD) and X-ray reflection (XRR) measurements
- Optical properties are determined by ellipsometry

Deposition and discharge characteristics

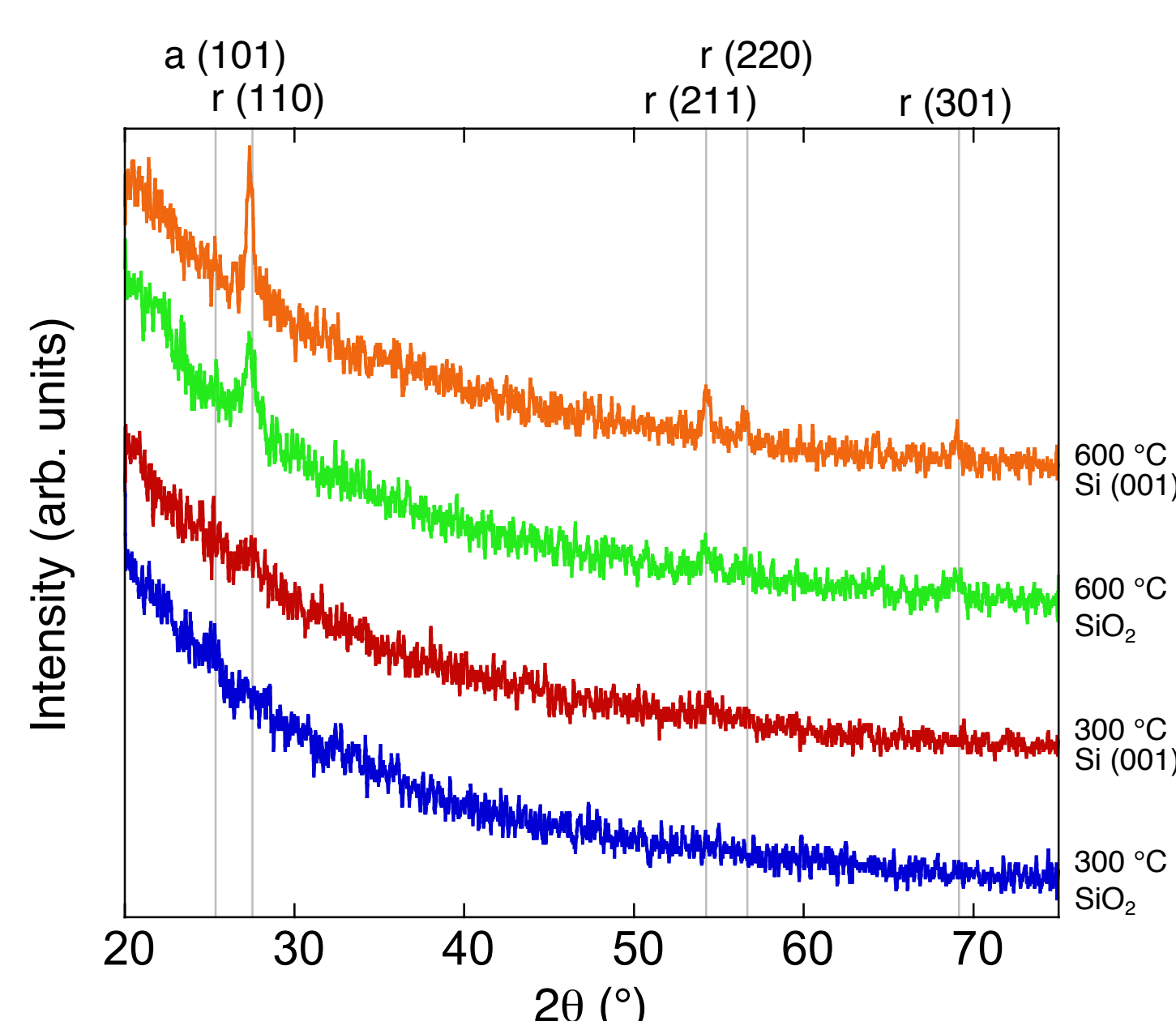
- HiPIMS
 - Square 530 V pulses
 - Pulse length 200 μs , repetition frequency 75 Hz,
 - Peak power density 0.7 kW/cm², average power 350 W
 - Ar/O₂(3.2%) gas mixture, total pressure 0.7 Pa
 - A distinct change in pulse shape is seen with the transition from metal to oxide mode \rightarrow plasma ignition is delayed but the peak current increases in oxide mode
 - All films were grown in metal mode with a growth rate of 0.3 Å/s resulting in a film thickness of 50–60 nm (measured by XRR and ellipsometry)
 - Grown simultaneously on Si(001) and amorphous SiO₂ (500 nm thermally oxidized Si)
- dcMS
 - Power 140 W
 - Ar/O₂(5.4%) gas mixture, total pressure 0.5 Pa
 - metal mode growth, growth rate of 0.6 Å/s resulting in film thicknesses of 100–120 nm (measured by XRR)
- 3 inch Ti target of 99.995% purity



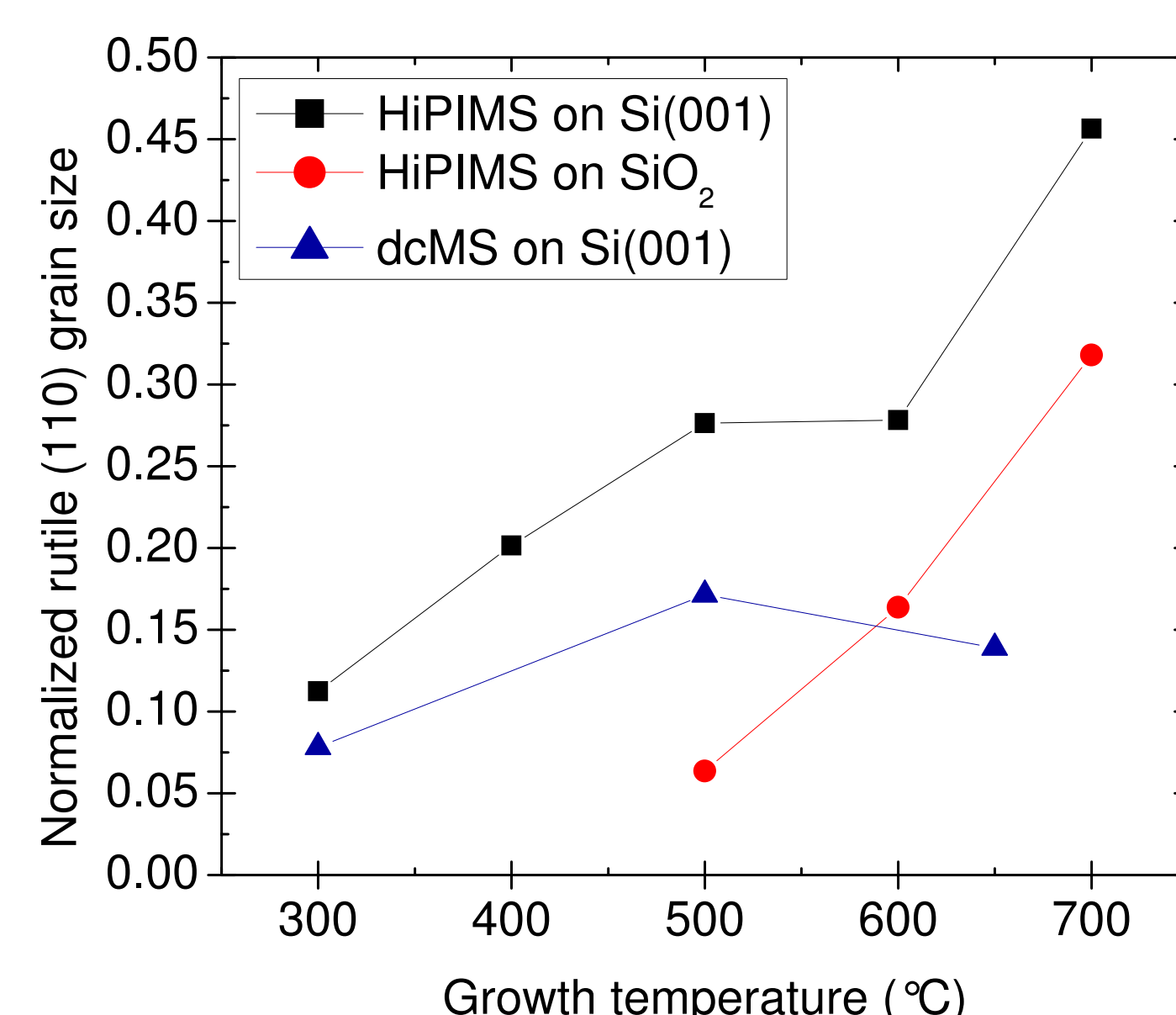
Pulse waveforms during metal and oxide mode. The voltage pulse is square and starts at $t = 0$. The pulse is cut short in oxide mode to limit the current

Phase composition

- GIXRD scans show that all the films are polycrystalline
- HiPIMS gives significantly larger grains than dcMS
- Growth on Si substrates promotes the nucleation of rutile grains and results in a larger grain size than when SiO₂ substrates are used
- Where diffraction peaks are visible they correspond to the rutile phase, except for the film grown on SiO₂ at 300 °C by HiPIMS where a small anatase peak is observed



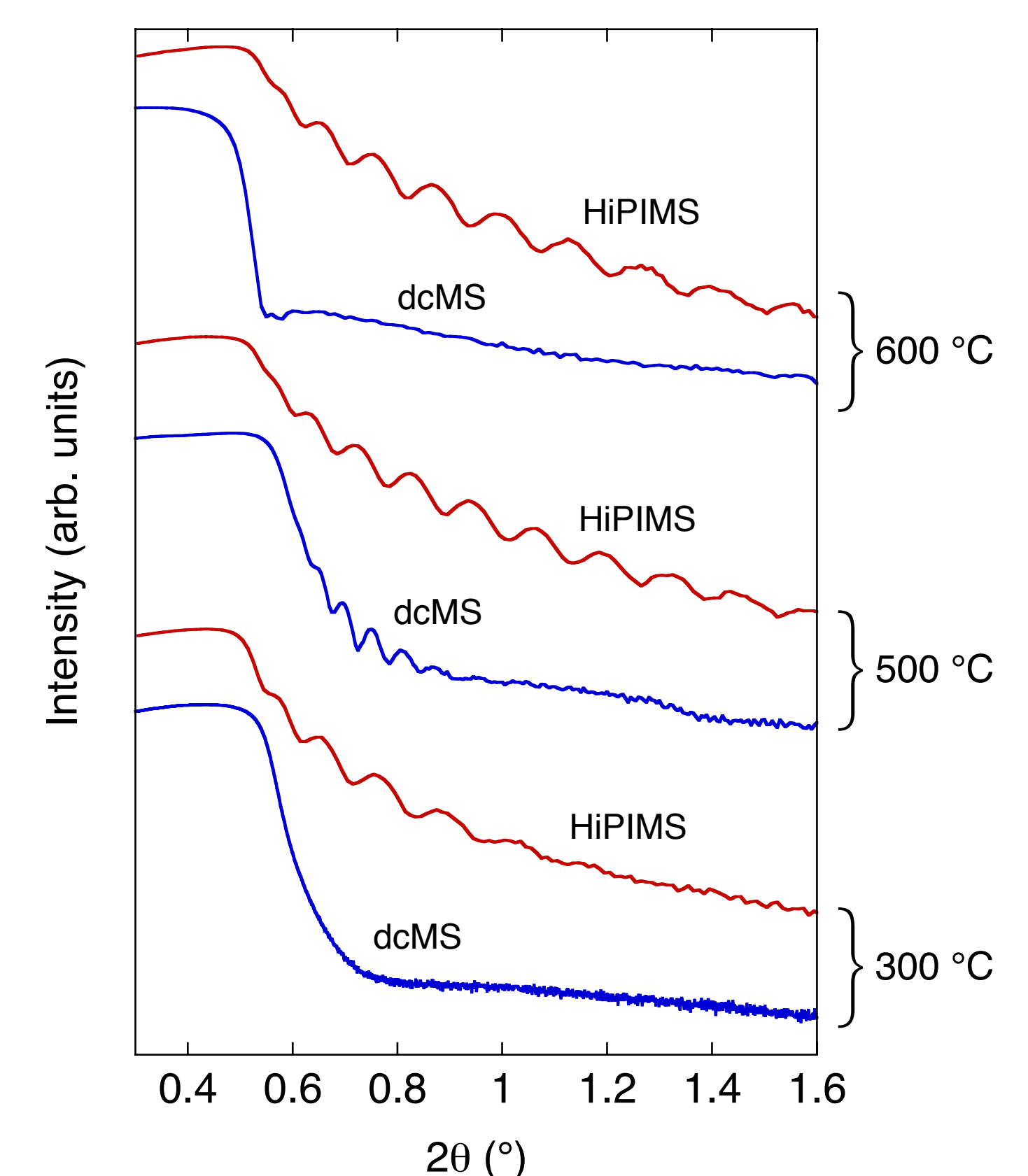
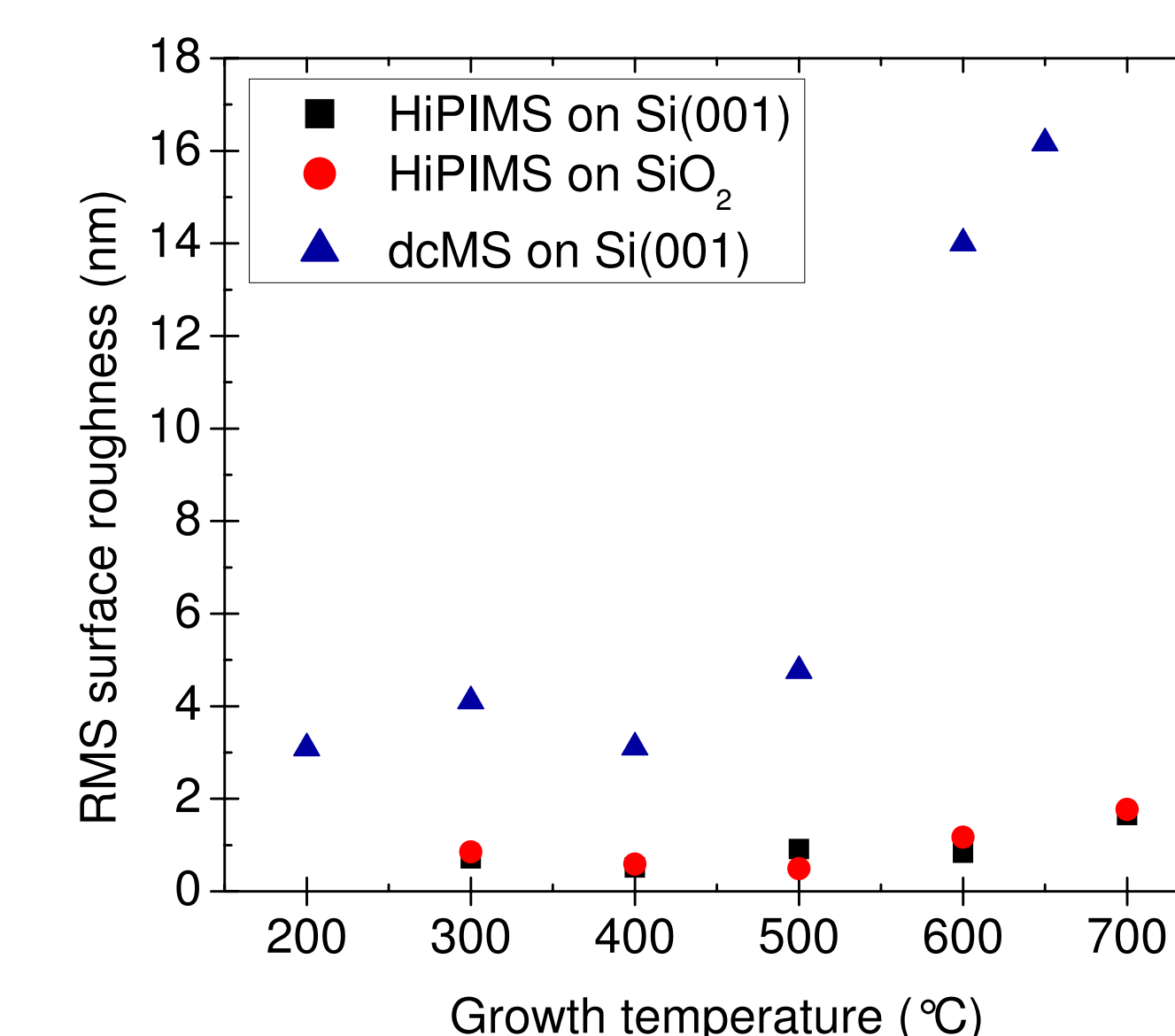
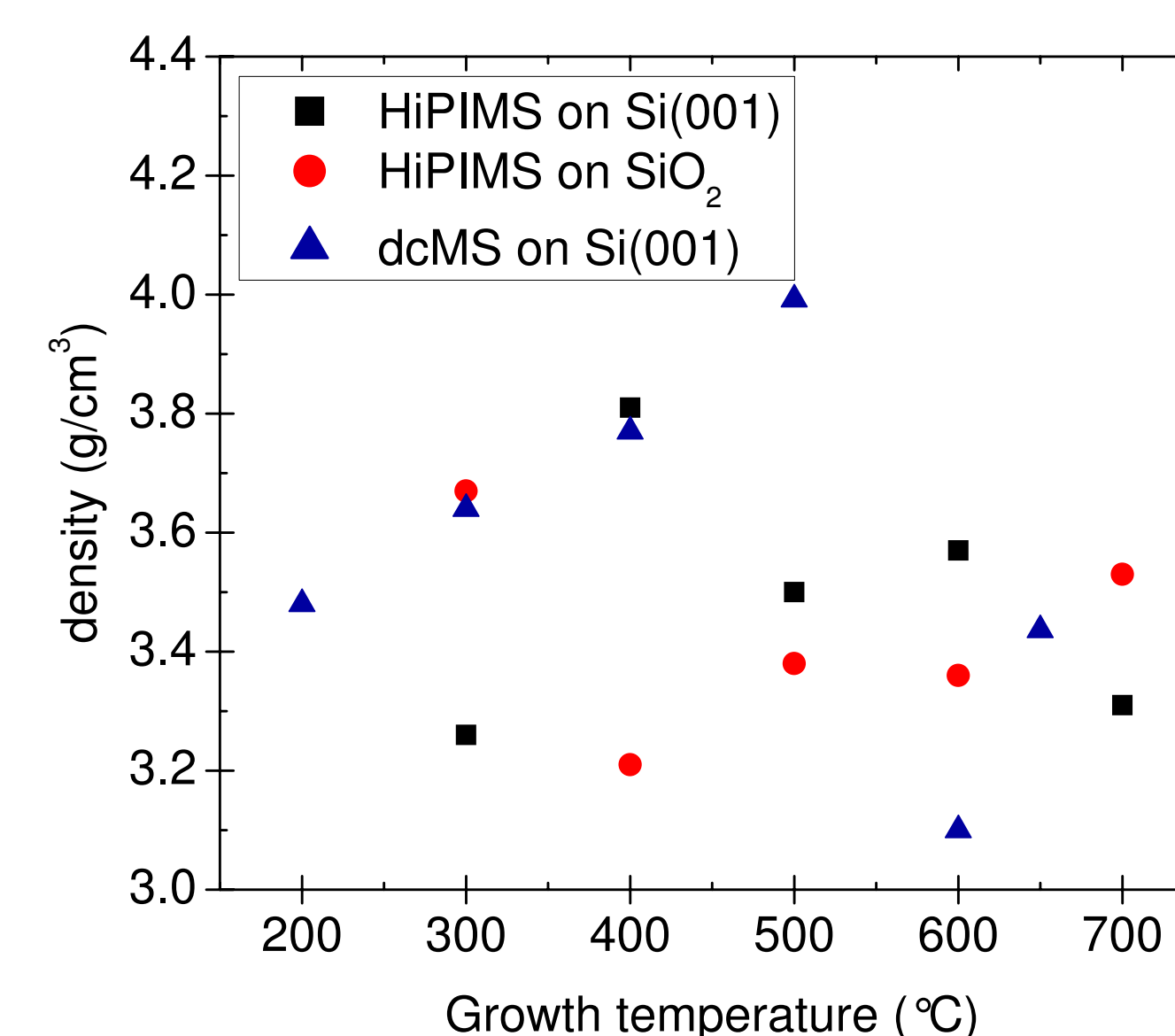
Grazing incidence x-ray diffraction measurements of HiPIMS-grown TiO₂ films



Rutile (110) grain size calculated from the FWHM of the (110) peak, normalized by film thickness

Roughness and density

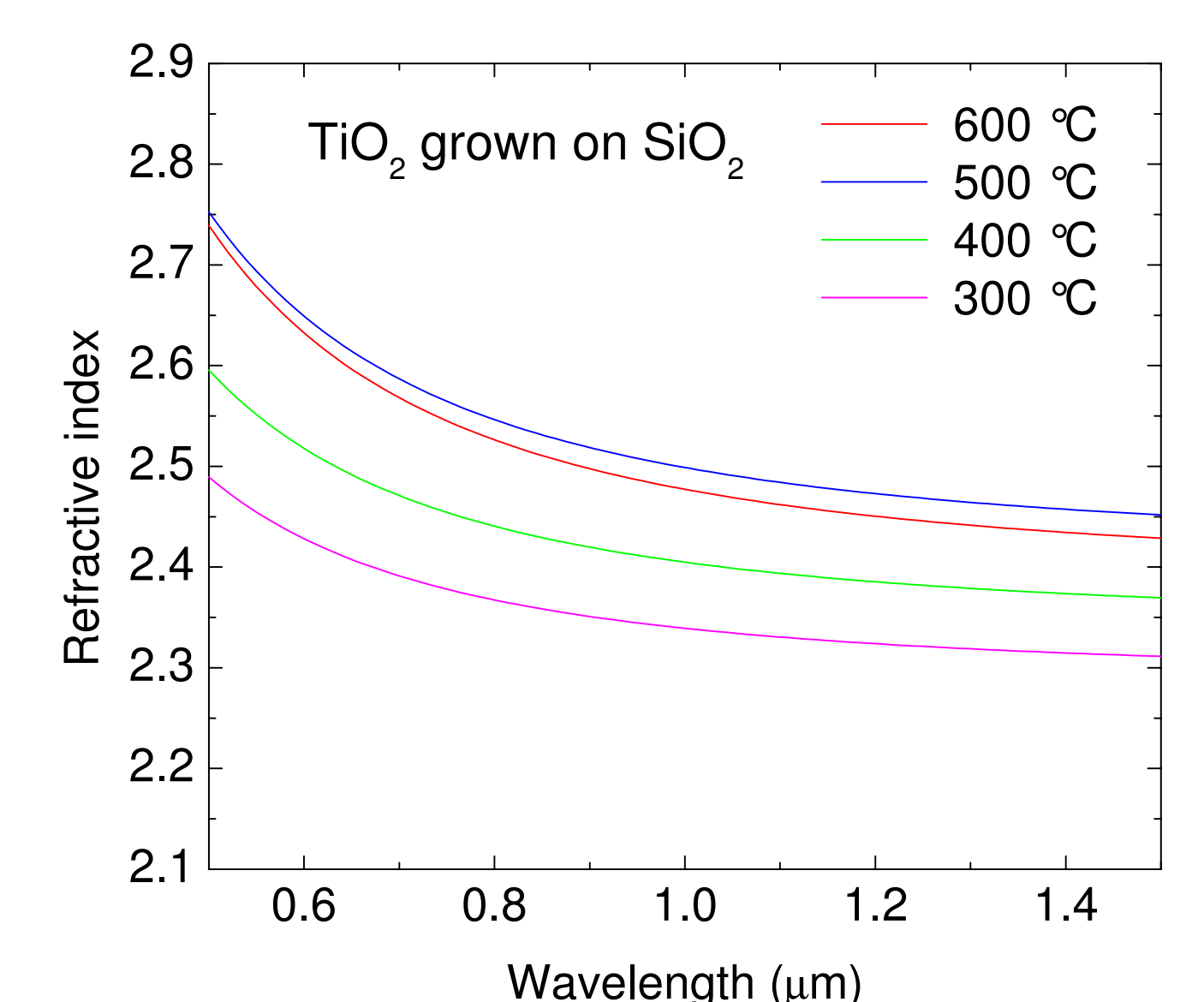
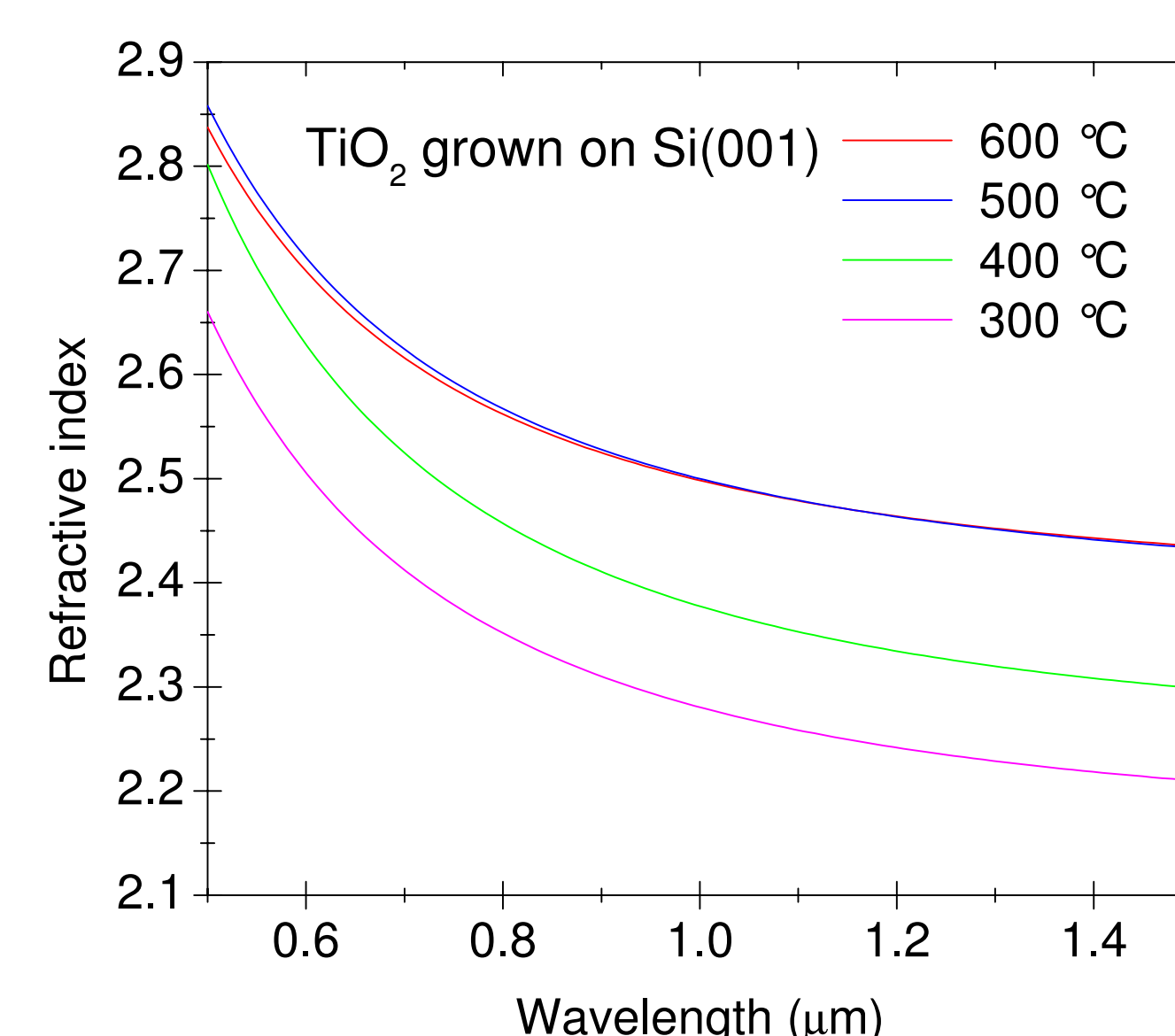
- XRR shows that films grown by HiPIMS have an order of magnitude lower surface roughness than films grown by dcMS
- Roughness increases with growth temperature
- Surface roughness is similar for Si and SiO₂ substrates
- Film density is lower than expected for rutile or anatase phases, despite large grain size \rightarrow indicates porosity
- No obvious trends observed in film density with growth temperature



X-ray reflection curves of HiPIMS and dcMS-grown films, including the surface roughness and density extracted from fitting

Refractive index

- Refractive index and film thickness measured by ellipsometry
- Refractive index of HiPIMS-grown films is well described by a simple Cauchy relation ($A+B/\lambda^2$) in the wavelength range 500–1500 nm
- Refractive index for dcMS grown films cannot be described by a Cauchy relation
- Refractive index varies with deposition temperature, is highest at 500–600 °C
- At 800 nm the refractive index is 2.56 for films grown at 500 and 600 °C



Conclusions

- HiPIMS produces rutile TiO₂ films with larger grains than dcMS in the temperature range studied (300–600 °C)
- The surface roughness is dramatically reduced in HiPIMS-grown films compared to dcMS
- HiPIMS produces optically transparent films with a high refractive index whereas dcMS-grown films show an anomalous variation in refractive index with wavelength

References

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- K. Sarakinos, J. Alami, S. Konstantinidis, Surface & Coatings Technology **204**, 1661 (2010).