Optical properties of the refractory metals at high temperatures

Mahima Arya[1], Gnanavel V. Krishnamurthy[2], Tobias Krekeler[3], Michael Störmer[2], Martin Ritter[3], Kjeld Pedersen[4], Alexander Yu Petrov,[1,2] Manfred Eich[1,2], Manohar Chirumamilla[1,4]

1. Institute of Optical and Electronic Materials, Hamburg University of Technology, Eissendorfer Strasse 38, Hamburg 21073, Germany.
2. Institute of Materials Research, Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research, Max-Planck-Strasse 1, Geesthacht 21502, Germany.
3. Electron Microscopy Unit, Hamburg University of Technology, Eissendorfer Strasse 42, Hamburg 21073, Germany.
4. Department of Materials and Production, Aalborg University, Skjernvej 4A, Aalborg 9220, Denmark.

E-mail: mch@mp.aau.dk

Thin film refractory metals play a crucial role in high temperature photonic/plasmonic applications such as thermophotovoltaics, thermoplasmonics and hot-electron applications [1,4]. However, the optical constants of these metals at high temperatures are unknown. Therefore, room temperature bulk single/poly-crystalline optical constants were used to calculate the optical response of the plasmonic/photonic structures at high temperatures, which leads to an uncertainty in estimating the device efficiency.

Herein, we present in-situ ellipsometry investigation of refractory metals (TiN, W, Mo and Ir [5, 6]) at high temperatures up to 1000 °C. Fig. 1 (a,b) shows the measured complex dielectric permittivities, real (ε_1) and imaginary (ε_2) parts, of these refractory metals at room temperature. The penetration depth of optical fields in these metals lies below 40 nm, and thin films with structural thicknesses of 80 nm or above exhibit the properties of semi- infinite samples. The complex dielectric permittivities of W, Mo and TiN are obtained by fitting a Drude-Lorentz oscillator model (equation 1), where conduction electron contribution and interband transitions are expressed by Drude and Lorentz terms, respectively.

$$\varepsilon(\omega) = \varepsilon_1 + i\,\varepsilon_2 \;=\; \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\Gamma_D\omega} + \sum_{j=1}^{N} \frac{\omega_{L,j}^2}{\omega_{0,j}^2 - \omega^2 - i\gamma_j\omega}$$

Here, ε_∞, ω_p, Γ_D, γ_j, are the background dielectric constant accounting for higher energy interband transitions outside the probed energy spectrum, plasma frequency, Drude damping and Lorentz oscillator damping factor, respectively. The optical constants of Ir are extracted using the wavelength-by-wavelength fitting method as no Drude-Lorentz model is accepted for it. At elevated temperatures, the electron–phonon interaction is the dominant mechanism leading to an increase of the electron collision frequency Γ_D. This increase is linear with the temperature and is independent of the film thickness. Further, we show experimentally the effect of film thickness on the optical properties, where the impact of the grain size due to grain-boundary and surface-scattering mechanisms is investigated.

We will present a detailed study on how the optical properties of the refractory metals change at high temperatures and thin films and define with it the efficiency of the refractory photonic/plasmonic devices.
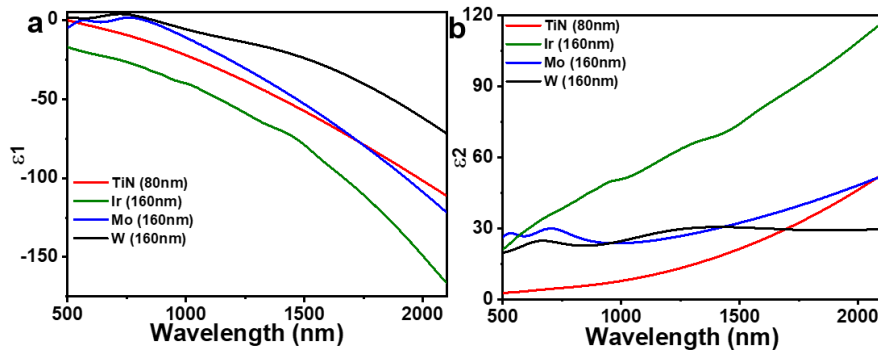

Fig. 1 a, b) Real and complex parts of the dielectric permittivities ε_1 and ε_2, respectively, of TiN, Ir, Mo and W thin films at room temperature.

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