Optical properties and surface characterization of PLD-grown Cu2ZnSnS4 by spectroscopic ellipsometry

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Citation (APA):
Optical properties and surface characterization of PLD-grown Cu$_2$ZnSnS$_4$ by spectroscopic ellipsometry

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Motivation

To apply spectroscopic ellipsometry on as-deposited Cu$_2$ZnSnS$_4$ films grown by pulsed laser deposition (PLD) at different temperatures (25-425°C) in order to:

- characterize topology and secondary phases at the surface
- extract the dielectric function of Cu$_2$ZnSnS$_4$ films

Preliminary analysis

- All films consist mostly of CZTS but are Cu- and Sn-rich (EDX)
- Documented inclusion of related secondary phases Cu$_2$SnS$_4$, SnS and Cu$_{2-x}$S (XRD, Raman)
- Improved crystallization at a higher temperature deposition temp. [°C]

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Raman spectra of 25°C film, focusing the laser at two different depths

- Except for at 425°C, there are two topographic layers: a smooth film (roughness < 2 nm) and sub-micron droplets
- At 425°C, larger crystal grains eliminate such a distinction (normal for hot substrate with PLD)
- With Raman spectroscopy, some secondary phases can only be detected if the laser is focused on top of the droplets (Cu$_{2-x}$S).
- Other phases can only be detected if the focus is at the film surface (Cu$_2$SnS$_4$)

Surface characterization

Conclusions

- When deposited at room temperature, the dielectric function of CZTS is of a Tauc-Lorentz type, typical of amorphous materials
- When deposition temperature is increased, the dielectric function exhibits more critical points, related to additional optical transitions
- Topographic features and surface phases can be detected by ellipsometry in some cases
- Ellipsometry can be used to confirm results of direct measurement techniques (SEM, AFM, Raman spectroscopy)

Acknowledgments

This work has been supported by a grant from the Danish Council for Strategic Research. CINF is funded by the Danish National Research Foundation (DNRF54).

Ellipsometry

Measurement side, angles of incidence, surface overlayer model, and dielectric function parametrization are selected individually for each film. The selection criteria are minimization of:

1. mean square error (MSE) of the fit
2. correlated errors of the parameters of interest
3. deviation from results of other measurement techniques

Comparison of parameter values obtained by ellipsometry and direct techniques

Real and imaginary part of the dielectric function of CZTS films

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