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Numerical Analysis of Temperature Calibration using Plasmon Energy Expansion Thermometry

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Background incl. aims

Transmission electron microscopy (TEM) has become an important tool for characterizing the microstructure in materials [1]. However, to gain access to the underlying structure-property relationships, real-time observations in TEM experiments are required to study the material's microstructure under operating or process conditions, e.g. at elevated temperature in in-situ heating experiments. And, with the advent of TEM nanoheaters that utilize microelectromechanical systems (MEMS) technology [2,3], atomic-scale studies at elevated temperatures became feasible.

However, the exact local temperature of a TEM sample itself remains rather uncertain, limiting the interpretation of observed structural phenomena observed in in-situ TEM heating experiments. Here, we explored how accurately plasmon energy expansion thermometry (PEET) [4] can be used to determine the local temperature.

Methods

As our model system, a tungsten (W) sample, prepared using a ThermoFisher Hydra plasma focus ion-beam (PFIB), was placed on a DENS Wildfire nanoheater [3]. For the PEET experiment, low-loss energy electron loss spectroscopy (EELS) was performed using ThermoFisher Spectra Ultra at 300kV with an energy resolution of 1 eV and a Gatan Continuum GIF with Dual-EELS functionality.

The site-specific temperature (T) within the W lamella was estimated by measuring the T-dependent energy shift of the W bulk plasmon in the low-loss EELS. The energy dispersion of 0.01 eV was used for an increased precision for detecting the plasmon energy shift.

To accurately estimate the temperature profile within the W lamellas with uniform sample thickness, we used the finite element method (FEM) in COMSOL. Further, the GPAW package [5] was used to simulate EELS spectra, based on the dielectric function. The temperature-dependent energy of the W bulk plasmon was estimated in the GPAW environment by implementing the temperature-dependent thermal expansion of the lattice constant.

Results

The COMSOL simulation models the heat flow and the temperature distribution in our W sample with increasing nanoheater temperature, providing an estimation to simulate corresponding low-loss EELS spectra. Our simulated EELS spectra using GPAW predicted a shift of the W bulk plasmon energy ΔE of ~0.236 eV when the temperature was increased from RT to 1000°C. The value of the simulated W bulk plasmon energy is at the same order of magnitude as our experimental PEET data (ΔE ~ 0.38 eV) when increasing the temperature from RT (25.11 eV) to 1000°C (24.73 eV) in our in-situ heating TEM experiment.

However, the deviation between our simulation and experiments indicated that more details need to be considered. One approach in the simulation is that the precision of PEET has been evaluated in our simulated EELS data from the uncertainties of the coefficient of thermal expansion and of the lattice constant at the reference temperature. Another reason could be that we have to take varying sample thickness into account in our COMSOL simulations.

Conclusion

Our study shows that PEET with W is able to measure local TEM sample temperatures in a quantitative way. The COMSOL/GPAW simulation can be used to predict the T-dependent plasmon energy and estimate the uncertainties for spectra in such experiments. This advances our approach in determining the local temperature across the sample in in situ TEM heating experiments.

Keywords:

Thermal expansion, EELS, PEET, Tungsten

Reference:

[1] K. Jungjohann et al., Transmission Electron Microscopy: Diffraction, Imaging, and Spectrometry (2016), 17-80. doi:10.1007/978-3-319-26651-0_2
[2] L. Mele, et al. Microscopy Research and Technique 79 (2016), 239-250. doi:10.1002/jemt.22623
[3] J.T. van Omme, et al., Ultramicroscopy 192 (2018), 14-20. doi:10.1016/j.ultramic.2018.05.005
[4] M. Mecklenburg et al., Physical Review Applied, 9, 014005 (2018). doi: 10.1103/PhysRevApplied.9.014005
[5] J. Mortensen et al., J. Chem. Phys. 160, 092503 (2024). doi:10.1063/5.0182685