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Machine Learning of In-situ Temperature Reconstruction from Metal-nanoparticle Thermometry on Transmission Electron Microscopy

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In-situ heating TEM have been widely employed to study thermodynamic behaviors at nanoscale. The temperature of TEM specimens are traditionally monitored macroscopically by thermocouples. Recently, various nanothermometers have been recently developed on TEM [1-7], enabling precise temperature imaging with nanoscale resolution. Converting observables into temperatures common require difficult manually analysis that cannot be completed while on the microscope. This limits design of experiments. With the development of artificial intelligence, it is possible to create fast-approximates of nanoscale temperatures on TEM. This study involves the temperature reconstruction of thermometrical images of nanoparticles using computer vision tools. The goal of this case study is to apply artificial intelligence / machine learning to analyze TEM images to reconstruct 2D temperature fields at nanoscale on TEM. The motivation comes from the concept of metal-nanoparticle thermometry which can record the highest temperature in the event and be read at a later time after the event is over [6,7].

Figure 1 shows a typical TEM image used for the demonstration. Single crystal silver nanospheres were deposited on TEM grids and heated under temperature gradients. The particle size changed with temperature, recording maximum temperatures experienced by the nanospheres. Temperatures were detected from TEM images based on a temperature-dependent size of crystal silver nanoparticles. By manually analyzing the location of dependent sizes of the nanoparticles, two-dimensional temperature fields were reconstructed in nanometer scale, as shown in Figure 1b. The spatial resolution of the temperature detection was 264 nm^2 or ~16 nm resolution in a linear direction.

In this work, the size and position of the silver nanoparticles are automatically measured using computer vision techniques [8-16]. Based on the temperature-depended size of those nanoparticles, temperature fields are reconstructed and plotted using plotting libraries for the Python programming language. Finally, a GUI is coded to package the analyses of the TEM images using Python Packages.

First, the areas for individual nanoparticle are calculated and stored in Comma-separated Values (csv) files containing the nanoparticle positions in x and y coordinates using Python OpenCV script. Assuming the nanoparticles are spherical. The area A of spheres recorded on TEM images is used to determine the radius r of the spheres which in turn calculate the diameter d of the nanoparticles. $r \approx 0.2821\sqrt{A}$, $d = 2r$.

Next, temperatures of the nanoparticles are calculated based on the relationship between the area of nanoparticles and the diameter of nanoparticles [6,7]. Figure 2a show the fitted temperature-diameter relationship from the reported data using Scipy open-source Python library. A trend-line analysis is performed with the reported data. It is determined that a logarithmic equation is best suited to approximate the relationship between diameter and temperature. Using the logarithmic equations in the

Python script, a scatter plot of 2D temperature fields was displayed, as shown in Figure 2b. Figure 2c shows one 3D plot of the temperature field from the pandas software library.

In order to pipeline this analysis for multiple TEM images and be convenient to users, a GUI program is created to calculate area and position, store measured data, and plot the reconstructed 2D temperature fields as well as to list diameter and position of individual nanoparticles. Figure 2d shows the interface.

In summary, utilizing Python programming language and third-party libraries, 2D temperature fields were reconstructed from TEM images demonstratively and a GUI was created. Local temperatures can be fast read on TEM at the nanoscale based on the nanoparticle thermometry. The Artificial Intelligence technique would speed up the in-situ heating TEM research and make real-time in-situ temperature monitoring possible at nanoscale [17].

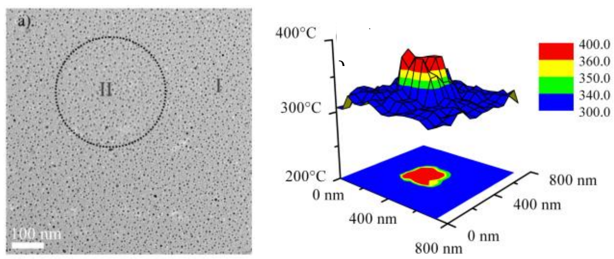

Figure 1: (a) A TEM image of nanoparticle thermometry and (b) manually reconstructed 2D temperature field from the TEM image. I region and II region of (a) were thermally exposed at low temperature and high temperature regions respectively. Source: Adapted from [6,7].

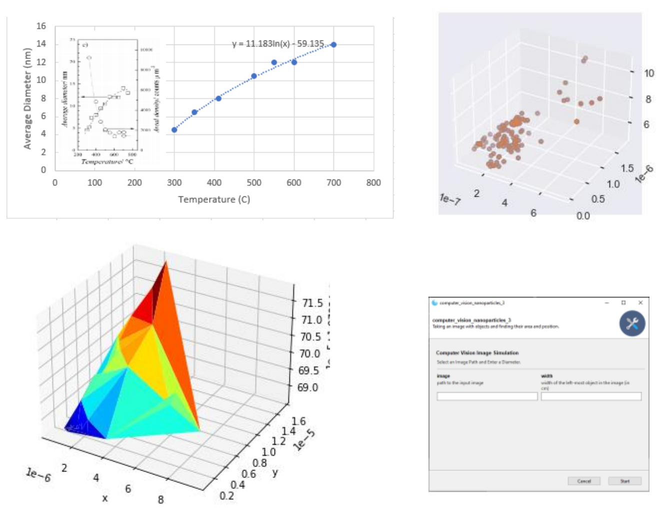

Figure 2. (a) Fitting curve of temperature-particle diameter relationship. Inset: reported temperature-size relationship [6,7]. 3D (b) scatter plot and (c) surface thermal image of reconstructed temperature field recorded on Figure 1a, showing temperature and locations of the nanoparticles in rectangular (x, y) coordinates. (d) GUI of Computer Vision Image Screen.

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References:

[1] Y. Gao, Y. Bando, Nature 2002, 415, 599.
[2] Y. B. Li, Y. Bando, D. Golberg, Z. W. Liu, Appl. Phys. Lett. 2003, 83.
[3] N. W. Gong, M. Y. Lu, C. Y. Wang, Y. Chen, L. J. Chen, Appl. Phys. Lett. 2008, 92, 073101.
[4] Y. C. Lan, H. Wang, N. Skula, X. Y. Chen, Y. L. Lu, G. Chen, and Z. F. Ren, Part. Part. Syst. Charact. 2015, 32, 65.
[5] M. J. Lagos and P. E. Batson, Nano Lett. 2018, 18, 4556.
[6] Y. Lan, H. Wang, X. Chen, D. Wang, G. Chen, and Z. Ren, Adv. Mater. 2009, 21, 4839.
[7] Chun, A. Tiny thermometers. Nature Nanotech (2009).
[8] A. Rosebrock, "Zero-parameter, automatic Canny edge detection with Python and OpenCV," Apr. 06, 2015.
[9] A. Rosebrock, "Measuring size of objects in an image with OpenCV," Mar. 28, 2016.
[10] R. Singh, "Computer Vision — An Introduction," Jun. 10, 2019.
[11] J. E. Byrd and D. D. Owens, J. Field Archaeol, 1997, 24, 315.
[12] Dana H. Ballard and Christopher M. Brown, Computer Vision. Prentice Hall, 1982.
[13] K. Reinhard, Concise Computer Vision. Springer, 2014.
[14] Linda G. Shapiro and George C. Stockman, Computer Vision. Prentice Hall, 2001.
[15] Tim Morris, Computer Vision and Image Processing. Palgrave Macmillan, 2004.
[16] Bernd Jähne and Horst Haußecker, Computer Vision and Applications, A Guide for Students and Practitioners. Academic Press, 2000.
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