Data mining approach for elucidating atomic-scale phenomena with transmission electron microscopy: A study of gold nanocontact

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In this study, we investigated structural deformation-induced properties of gold nano-contacts (Au-NCs) with applications of machine learning on mining the data of three synchronous time-series, i.e., (i) transmission electron microscopy (TEM) images, (ii) the corresponding elastic spring constant and (iii) electrical conductance [1]. In the initial stage of preprocessing, we used a deep image segmentation [2] model to automatically extract the contact regions captured in the TEM images. To coherently characterize the Au-NC, we designed 13 structural features which were then used by non-linear regression models [3] to predict for the elastic spring constant and conductance. The high accuracy in prediction can demonstrate for descriptiveness of the designed structural features. Further incorporating these features into a regression-based metric learning model [4], we constructed a two-dimensional map embedding characteristic information of contact structure with regard to the elastic spring constant. On the learned map, we grouped Au-NCs with characteristic shapes and analyzed the correlations between those shapes and physical properties. Furthermore, we implemented a generative adversarial network (GAN) [5] and used its capability of generating realistic images as a mean to conduct virtual experiments. Specifically, hypothetical TEM images of Au-NCs under various actuating conditions of pulling/pushing were generated for a better recognition of Au-NC structural transformation behaviors. The efficiency of GAN model can be qualitatively verified with shape-properties correlations as extracted from the metric learning map. As a result, the effects of actuating conditions were visually exhibited, which elaborates consequent changes in Au-NC structural factors, especially atomic rearrangement, and in physical properties at the nanoscale.

References

[1] K. Ishizuka, M. Tomitori, T. Arai, and Y. Oshima, Applied Physics Express **13** (2020).
[2] O. Ronneberger, P. Fischer, and T. Brox, in International Conference on Medical image computing and computer-assisted intervention (Springer, 2015) pp. 234-241.
[3] K. P. Murphy, Machine learning: a probabilistic perspective (MIT press, 2012).
[4] K. Q. Weinberger and G. Tesauro, J. Mach. Learn. Res.**2**, 612 (2007).
[5] T. Karras, T. Aila, S. Laine, and J. Lehtinen, in International Conference on Learning Representations (2018).