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Direct prediction of electrical properties of grain boundaries from photoluminescence profiles using machine learning

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Kentaro Kutsukake,[1,a)] Kazuki Mitamura,[2] Noritaka Usami,[2] and Takuto Kojima[3]

AFFILIATIONS

[1]Center for Advanced Intelligence Project, RIKEN, Tokyo 103-0027, Japan
[2]Graduate School of Engineering, Nagoya University, Nagoya 464-8603, Japan
[3]Graduate School of Informatics, Nagoya University, Nagoya 464-8603, Japan

[a)]Author to whom correspondence should be addressed: kentaro.kutsukake@riken.jp

ABSTRACT

We present a machine learning model to directly predict the carrier recombination velocity, v_{GB}, at the grain boundary (GB) from the measured photoluminescence (PL) intensity profile by training it with numerical simulation results. As the training dataset, 1800 PL profiles were calculated with a combination of random values of four material properties—v_{GB}, the GB inclination angle, and the carrier diffusion lengths in the grains on both sides of the GB. In addition, the measured noise was modeled artificially and applied to the simulated profiles. A neural network was constructed with the inputs of the PL profile and the outputs of the four properties. This served as the solver of the reverse problem of the computational simulation. The coefficient of determination and the root mean squared error of v_{log}, which is the common logarithm of v_{GB}, for the test dataset were 0.97 and 0.245, respectively. This prediction error was sufficiently low for the practical estimation of v_{GB}. Moreover, the calculation time was reduced by a factor of 198 000 compared to conventional numerical optimization of repeating the computational simulations. By utilizing this fast prediction method, continuous evaluation of v_{GB} along a GB was demonstrated. The finding is expected to advance scientific investigation of the electrical properties of local defects.

Experimental measurements are generally performed on materials to determine their properties, such as electrical, optical, magnetic, and mechanical properties. In some cases, the desired property may not be determined directly from the measurement data. In such cases, computational simulations that model the physical and measurement systems are used to determine the material properties. Figure 1(a) shows a schematic of the process for evaluating the electrical property of the grain boundary (GB) through carrier and optical simulation using photoluminescence (PL) image measurement as an example. A computational simulation solves the governing equations and yields a spatial distribution of the excess carrier density. The physical properties are incorporated into the model as parameters of the governing equations and boundary conditions. Subsequently, a measurable PL intensity profile is calculated from the distribution of the carrier density by simulating the luminescence and measurement systems. Thus, if the series of simulations is handled as a function, the inputs are the physical properties and the outputs are the measurable PL intensity profiles.

To assess the physical property values from the measurement data, the reverse problem of the simulations must be solved. Generally, this reverse problem is solved by optimizing the simulation output onto the measurement data. Many optimization methods are used to evaluate material properties, including the gradient method,[1–3] genetic algorithm,[4] and Bayesian optimization.[5] However, these optimization methods require repeated calculations of the simulations, which increase the calculation costs.

Recently, machine learning (ML) has been applied to materials research simulations. One application is a surrogate model[6] for high-cost computational simulations, such as computational fluid dynamics simulations,[7–13] electric carrier simulations,[14,15] and atomic-scale simulations.[10,16–18] In these applications, the inputs and outputs of the machine learning model correspond to those of the computational simulations. Thus, faster computation is a major advantage of the surrogate model using machine learning. Another application of machine learning is to solve the reverse problem of simulations directly. Several researchers have reported machine learning