An Intelligent Prediction Model to Increase Reliability for Electrochemical Production of High-Quality Graphene

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Abstract

The reliability of graphene manufacturing usually consists of two consecutive steps of graphene production and functionalization, which are mainly accompanied with several reaction routes and waste generation [1]. Herein, we demonstrated a facile one-step method for the simultaneous exfoliation of graphite and surface functionalization of the resulting graphene using electrochemical approach. In this study, we showed that presence of a water-soluble acrylate monomer e.g., *n*-butyl acrylate in an ammonium sulphate electrolyte solution can functionalize graphene through in situ polymerized *n*-butyl acrylate monomers during electrochemical exfoliation. We identified and optimized the key parameters (electrolyte concentration, acrylate monomer concentration, and applied voltage) which are involved in quality of graphene nanosheets (thickness and yield) by constructing an intelligent prediction model [2,3].

To build an accurate model, sufficient amount of data is needed. Due to the cost, time consuming, accuracy of experimental data, the following steps with small experimental samples are proposed: (1) Design of Experiment (DOE), (2) precise selection and developing a model; (3) validating the developed model; and (4) performing optimization based on the validated model (see Figure 1 (c)).

Based on the result of intelligent prediction model (see Figure 2 and Table 1), the optimum condition of overall yield for electrochemically synthesized and functionalized graphene nanosheets is ~25% with respect to as-received natural graphite, and at least 80% few-layer nanosheets with a thickness less than 7 nm.

Table

Table 1: Prediction Model Validation Results

CVE	SEP	RMSE
12.66487	4.70403	9.64365

References

[1] Omid Zabihi, Scientific Reports, 6 (2016) 3560.

[2] H.Khayyam, et al., Limited Data Modelling Approaches for Engineering Applications, Nonlinear Approaches in Engineering Applications (2018)345-379.

[3] H.Khayyam , et al. Dynamic Prediction Models and Optimization of PAN Stabilization Processes for Production of Carbon Fiber, IEEE Transaction on Industrial Informatics (2015) 887-896.

Figures

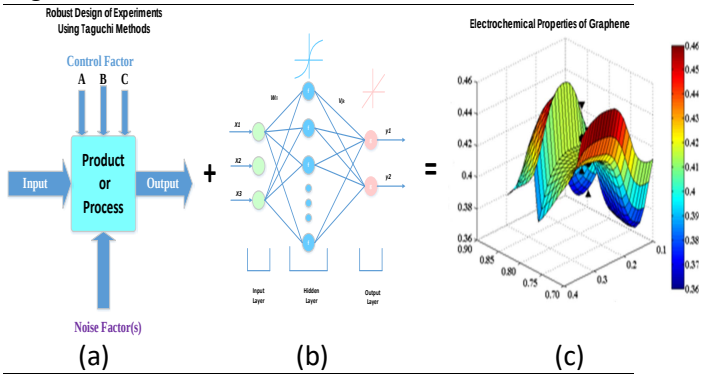

Figure 1: Intelligent Prediction Model:(a)Taguchi DOE, (b) ANN training, (c)prediction model.

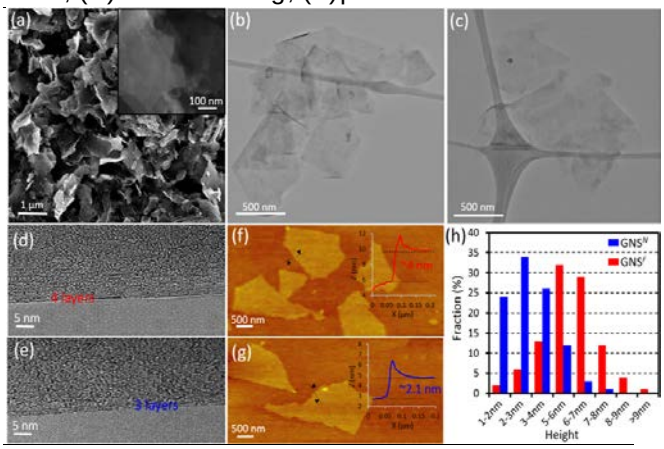

Figure 2: Optimal electrochemical condition for graphene production: (a)SEM, (b-e) TEM, and (f-h)AFM results.