弱電離プラズマ中の複雑化学反応ネットワークの可視化（Ⅲ）

Visualization of complex chemical reaction networks in weakly-ionized plasmas (III)

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1. Introduction

Weakly-ionized plasmas, playing various roles in industrial material and biochemical processes with sufficient and stable technological outputs, include chemical-reaction complexities that are outstanding in comparison with other chemical processes. In parallel, information technology rapidly grows in its increasing categories of applicable targets, and a number of concepts and techniques are currently available for analysis on complicated phenomena that cannot be treated by simple principles in conventional methods. In this report, we perform community detection in complex chemical reactions in weakly-ionized plasmas, which is based on network analysis and graph theory, followed by our previous reports [1-3].

2. Analytical Methods

We study silane (SiH_4) plasmas in which hundreds of chemical reactions take place among tens of such species as radicals, ions and electrons. We simplify one reaction using directed edges that start from nodes representing agent species in a given reaction equation and end at those of product species (Fig.1(a)) [1,3]. Thus, a complex network in the form of a graph is created (Fig.1(b)), and we classify species into a few *communities* in which the belonging species are linked closely; community detection is now being intensively studied in the scientific category of complex networks [4].

3. Analytical Results

For community detection, here we show a result after the procedure based on edge betweenness [4]. As in shown in Fig. 1(b) and Fig. 2, besides small groups, we find two large communities; one community includes SiH_4, SiH_3, Si_3H_8, and electrons (for thin-film deposition), and another contains SiH and higher-order radicals (for polymerization and particle formation).

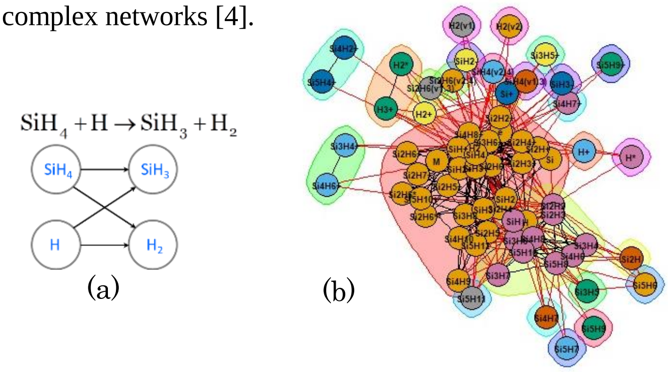

Fig. 1. (a) Example of nodes and edges for one chemical reaction [1], and (b) chemical reaction network in SiH_4 plasma [1] with community partitioning.

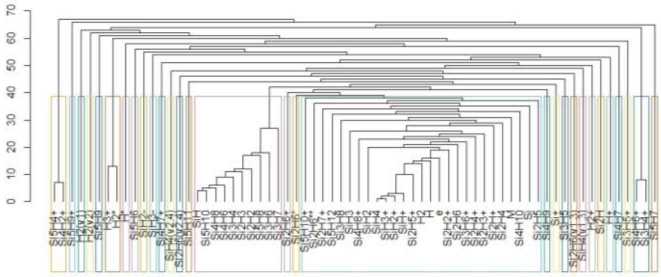

Fig. 2. Dendrogram based on edge betweenness calculated from network topology in Fig. 1.

References [1] Y. Mizui *et al.*, Symmetry **9**, 309 (2017). [2] O. Sakai *et al.*, AIP Advances **5**, 107140 (2015). [3] Y. Mizui *et al.*, *Complex Networks VIII* (Springer International Publishing, Cham, 2016), pp. 135-140. [4] E. D. Kolaczyk, *Statistical Analysis of Network Data: Methods and Models* (Springer, Berlin, Germany, 2009).

