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（Ⅱ）

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

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1. Introduction

Weakly-ionized plasmas play various roles in industrial material and biochemical processes with sufficient and stable technological outputs, and their scientific principles are being investigated by many researchers for their expanding applications, where their complexities 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 investigate a method for macroscopic understandings of 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) and methane (CH_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)). Thus, a complex network in the form of a graph is created (Fig.1(b)), and we can calculate various centrality indices for each node or species that is in statistical properties of the network.

3. Analytical Results

In addition to visualization for microscopic views [1,2], we propose a distribution histogram of species counting along central indices such as betweenness (C_b) and closeness centralities [1], as shown in Fig. 2. In this diagram, the C_b values indicate importance as intermediates. In comparison with distributions of random graphs, those for silane and methane have broad spectra, which can be called *semi-scale-free* properties. These results indicate that complexities in plasma chemistry include robustness for environmental effects with various roles in network topology.

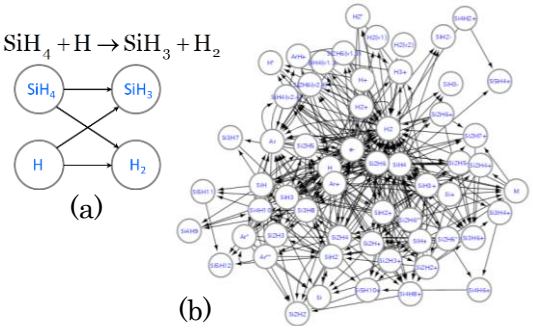

Fig. 1. (a) Example of nodes and edges for one chemical reaction [1], and (b) chemical reaction network in SiH_4 plasma [1].

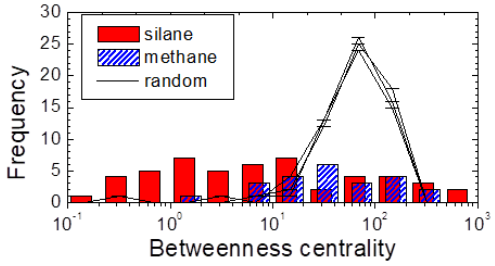

Fig. 2. Distribution of species number along betweenness centrality index (C_b) for network in Fig. 1 and others in comparison [1].

References [1] Y. Mizui, T. Kojima, S. Miyagi and O. Sakai, 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.