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

Visualization of complex chemical reaction networks in weakly-ionized plasmas

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1. Introduction

Although weakly-ionized plasmas play various roles in industrial material and biochemical processes with sufficient and stable technological outputs, their scientific principles are being still investigated by many researchers, partly due to their extreme complexity. 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 this report, we investigate a method of intuitive understandings of complex chemical reactions in weakly-ionized plasmas, which is based on network analysis and graph theory and 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. Thus, a complex network in the form of a graph is created, as shown in Fig.1, and we can calculate various centrality indices for each node or species that is in statistical properties of the network.

3. Analytical Results

One graphical visualization we have proposed so far is a diagram with betweenness (C_b) and closeness (C_c) centrality indices [1], as shown in Fig. 2. In this diagram, the C_c values with similar C_b indicate the degree between agents and products, and C_b implies importance of intermediates. We also observed semi-scale-free properties in the C_b distribution in both SiH_4 and CH_4 networks. These results indicate that this visualization is useful for display of both macroscopic properties of network and microscopic insights of individual species.

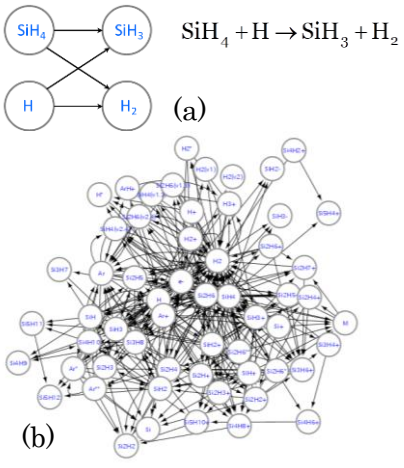

Fig. 1. (a) Example of nodes and edges for one chemical reaction [1], and (b) chemical reaction network in SiH_4 plasma [1].

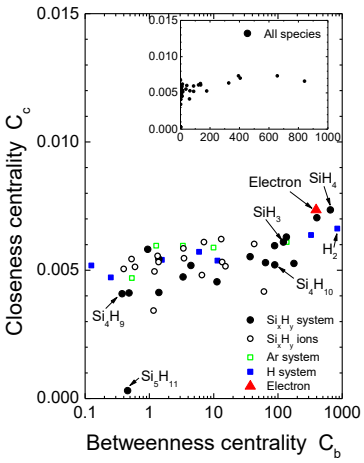

Fig. 2. Diagram of betweenness and closeness centrality indices for network in Fig. 1 [1].

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.