Mathematical analysis to clarify how reaction networks grow in plasmas

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Abstract: It is becoming increasingly important to understand and predict the nature of complex chemical reactions induced by plasmas. In this study, we develop complex network analysis based on mathematical graph theory to understand how chemical reaction networks grow in plasmas, how plasmas are formed, and how they are stabilized.

1. Introduction

Network analysis based on mathematical graph theory has been applied in various fields, including physics, chemistry, biology, computer science, geography, economics and sociology [1,2]. In the field of plasma science and technology, understanding the nature of complex chemical reaction systems is of importance. The network analysis enables us to reveal the hidden feature of its complexity. Recently, the basic characteristics of gas-phase plasma chemistry has been examined [3,4]. The growth mechanism of the plasma chemical network contains important features for understanding how a plasma forms itself and how it stabilizes itself. In this work, we propose a theoretical model to analyze how plasma chemical networks grow.

2. Methods

In graph theory, the elements and the interactions between these elements of the system are represented as nodes and edges, respectively. When we apply the graph theory to the plasma chemistry, the nodes correspond to species and the edges represent the connections among species in the reaction kinetics [3,4]. To capture the growth process of plasma chemistry network, the growth transition diagram has been developed.

3. Results and Discussion

Figure 1 shows the degree diagrams of the reaction network in the helium+oxygen+nitrogen plasma [5]. Species which act as hubs are shown as large node circles and are located in the center region. The major reaction paths are shown as thicker edges. It is clearly visualized that the network grows and the chemistry becomes richer during the generative process from (a) to (f), *i.e.* the new nodes join the network and link edges. In the early stage (from (a) to (d)), the electrons occupy a key position in the diagram, which suggests that the high-energy electron-driving process initiates the network generation system. Other background species, such as helium atom, oxygen molecule and nitrogen molecule are located at the center region of the diagram in the maturation stage (from (d) to (f)). These species are the cause of various dissociations, excitations, and ionizations, and the diversity of such reactions is also a characteristic of plasma. The statistical analysis also suggests that the preferential attachment and scale-freeness are key features in the growth of plasma reaction networks, which are the essential factors for stable networks.
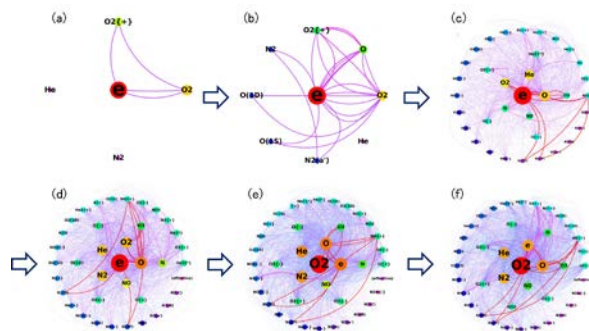
Fig. 1. Growth transition diagram to visualize the generation process of the reaction network in a He+O_2+N_2 plasma (from (a) to (f)).

4. Conclusion

The proposed mathematical approach has provided valuable insights into complex reactive systems. These findings can shed light on how different plasma species interact and what reactions they trigger. Graphical and theoretical analysis allows us to understand not only the unique properties of certain steady states but also transition properties that may be common to different plasma networks.

References

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