

**Graduate Physics Seminar
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FULLERENE MODELING

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Abstract

The molecules from fullerene family are rapidly becoming a part of our daily lives due to the wide range of their unique properties and extensive field of their potential applications. High demand for these materials revealed a necessity to understand the process of fullerene growth in order to optimize their production. Since the fabrication technique has a large influence on the material properties, several methods have been suggested.

The focus of this presentation will be electric-arc discharge method, where fullerenes are formed by vaporizing graphite electrodes in low pressure gas atmosphere. The detailed understanding of growth mechanisms in arc discharge reactor requires the development of a mathematical model that approximates the physical behaviour of non-equilibrium plasma coupled with a nonlinear chemical systems.

In this presentation several such models from various authors (Bilodeau, Farhat, Alekseev) are presented along with chemical kinetics model (Scott), that describes nucleation and growth of carbon clusters and fullerenes.