第12回拠点セミナー（構造材ゼミ 019）
マテリアルズインテグレーションの実現に向けて

From The Center for Hierarchical Materials Design to a New Tool for Materials Simulation

presented by

Prof. Peter W. Voorhees

Northwestern University, US

日時： 2016年3月1日 (火曜日) 13:00 – 14:00

場所： 千現地区 先進構造材料研究棟 5階 カンファレンスルーム

主催： 構造材料研究拠点

問い合わせ先： 門平卓也 （マテリアルズ・インフォマティクスプラットフォーム）

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講演者： Prof. Peter W. Voorhees (Northwestern University, US)
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講演概要：

The classical materials creation process involves a laborious procedure wherein intuition drives the design of a material that is then created, and tested. In most cases, the design goals are not attained, and this costly procedure is repeated. The Materials Genome Initiative (MGI) seeks to replace this process and thus bring innovative new materials into commercial applications faster and at a lesser expense. To attain the goals of the MGI, our newly formed Center for Hierarchical Materials Design will develop verified codes and curated databases that will enable proliferation of both a materials-by-design strategy and materials discovery. An introduction to the center will be given. Phase field crystal (PFC) models is one of the computational tools under development. It provides insight into the atomic scale motion and defect formation to be determined on diffusive timescales. Using the PFC approach, the structure and dynamics of grain boundaries have been examined. We find that the atomic-scale structure of the boundary gives rise to qualitatively new grain growth kinetics as well as to both grain rotation and translation. The grain translation is a result of the climb, glide, and interactions of the dislocations that comprise the grain boundary, as well as dislocation interactions at trijunctions. The effect of temperature and vacancy concentration on grain boundary structure, migration, and grain-boundary pinning will also be discussed.

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