Kinetic Monte Carlo Study on Crystal Growth

Project Proposal

Introduction

Computer simulation serves as a powerful tool to study dynamic physical processes. Due to the complex nature of solid-liquid phase transition, it is usually more applicable to apply theoretical models via simulations to understand the dynamical details of crystal growth under melt. One such model involves kinetic Monte Carlo (KMC) scheme to treat the growth process as a stochastic process. Despite its successful implementation on alloys, we would like to investigate the transferability of this model to sugar alcohols, which are very promising materials for future long-term heat storage industries.

Tasks

1. Understand the theory of KMC
2. Improve the KMC code
3. Use key parameters to tune the KMC model and examine its transferability to sugar alcohols
4. (Bonus) Improve the code to include more complicated conditions and anisotropic effects

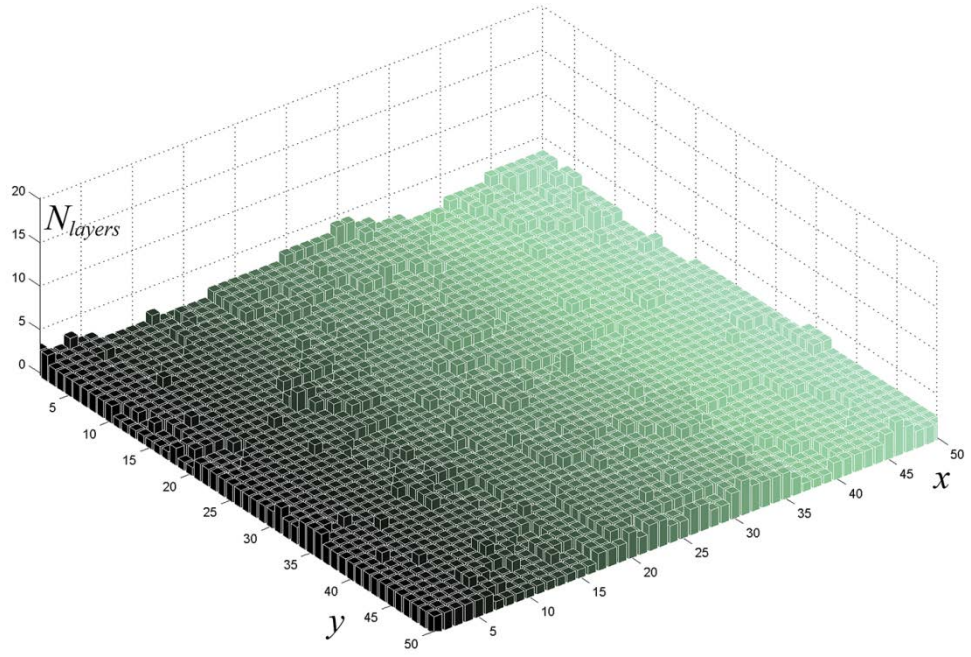

Figure. A dynamic evolvement of a growing crystal surface represented by cubic lattices

Reference

[1] M. Rak, M. Izdebski and A. Brozi, *Computer Physics Communications* 138(**2001**) 250-263

Contact: Dr. Silvia V. Nedea, s.v.nedea@tue.nl, GEM-Z 2.122

/Energy Technology / Department of Mechanical Engineering