Numerical simulations of the growth of graphene on Cu (111)

P. Gaillard, T. Chanier, P. Moskovkin, L. Henrard, S. Lucas

University of Namur, Research center for the Physics of Matter and Radiation (PMR), 61 Rue de Bruxelles, B-5000, Namur, Belgium

stephane.lucas@fundp.ac.be

Abstract

Graphene is a material that has attracted a great deal of attention recently, through its exceptional electric, optical and mechanical properties. Foreseen applications such as transparent conducting layers or sensors depend on growing large areas of crystalline graphene with controlled quality. Chemical vapour deposition is the most promising method to reach this goal, but improving film quality requires a better understanding of film growth.
This work presents the modelling of the growth of a graphene film on Cu (111) through the use of kinetic Monte Carlo (KMC) simulations, through a program that is described in [1]. These simulations require the knowledge of activation energies for the more stable adsorption sites and of the diffusion barriers between those sites. Based on detailed parameters obtained from ab-initio simulations, larger scale KMC simulations were performed as a function of the carbon partial pressure and the temperature.
We studied the grain size and shape of graphene as a function of the carbon partial pressure and of temperature. In particular, we focussed on the conditions of the formation of grain boundaries when two graphene crystallites merge.
The figure shows an example of a simulation of graphene growth on copper by CVD. The grey dots are carbon atoms, and the orange dots represent the hexagonal graphene lattice with additional “bridge” sites included.

References

[1] S. Lucas, P.Moskovkin, Thin Solids Films, Volume 518, Issue **18** (2010), Pages 5355-5361.

Figures