



Contribution ID: 150

Type: Oral

Machine learning for Cu surface kinetic Monte Carlo

Thursday 19 September 2019 18:40 (5 minutes)

Kinetic Monte Carlo (KMC) is among the most efficient methods for modelling diffusion. In the context of CLIC, we're interested in the diffusion processes on the Cu surface - especially under high electric fields that are present prior to electric breakdown events.

The accuracy of a KMC model relies on the comprehensiveness of the catalogue of different migration events that are available for the simulated system, and on the accuracy of the energy barriers associated with those events. The heavy calculations required to find the energy barriers are typically the bottleneck of KMC simulations.

We are improving the KMC model earlier developed in our group, by adding nuance to the way we describe the atomic environments of the migration events, with the aid of machine learning. At the moment the machine learning model has reached performance level comparable to the currently existing one, but we hope that we can eventually capture physical processes more realistically. In this talk, we will present some of the newest simulation results obtained with the machine learning KMC model, as well as some outlook on future work.

Primary authors: KIMARI, Jyri; JANSSON, Ville (University of Helsinki); VIGONSKI, Simon (University of Tartu); BAIBUZ, Ekaterina (University of Helsinki); Dr DOMINGOS, Roberto (Rio de Janeiro State University); ZADIN, Vahur (University of Tartu (EE)); DJURABEKOVA, Flyura (Helsinki Institute of Physics (FI))

Presenter: KIMARI, Jyri

Session Classification: Poster

Track Classification: Modeling and Simulations