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Artificial neural networks for Cu surface migration barrier prediction

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Diffusion is a slow process compared to atomic vibration. It is thus inefficient to simulate using methods that work in that short time scale, such as Molecular Dynamics. Substituting the chaotic motion of individual atoms with discrete jumps between potential energy minima yields an efficient and widely used method that is Atomic Kinetic Monte Carlo (AKMC). Each jump has a rate Γ determined by its energy barrier E_m and temperature T:
\begin{equation}
\Gamma \propto \exp\left(-\frac{E_m}{k_BT}\right)
\end{equation}

The weakness of AKMC is the requirement for the knowledge of the energy barriers associated with each jump. Accuracy of the simulation can be improved by allowing new types of jump events, and calculating their barriers, until the number of required barriers grows unfeasibly high.

An alternative way to approach this trade-off between accuracy and affordability is to cut corners with machine learning. A subset of jumps can be sampled from the entire configuration space, and an artificial intelligence can be taught to interpolate and extrapolate as necessary during the AKMC simulation.

In this work, Artificial Neural Networks (ANN) have been used to learn and predict Cu surface migration barriers. The ANN barrier predictor method has been implemented in an AKMC code Kimocs, developed earlier in our group. The results this far will be described in this presentation. The long-term goal of the project is to model the Cu surface under electric field more accurately than before, to study the phenomena that take place in Cu structures such as those of the Compact Linear Collider.

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