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ABSTRACT

The Connection between the Microscopic Energy Landscape and the Macroscopic Activation Energy

S. Neitzel-Grieshammer[1]

[1]FH Münster – University of Applied Sciences, Steinfurt, Germany

Ionic conductivity in solids is the key property for various applications, including batteries, fuel cells, and sensors. The ionic conductivity depends on the concentration of charge carriers and their mobility, which itself depends on the activation energy. While the effect of the charge carrier concentration is limited, variations in the activation energy EA can significantly affect the transport kinetics.

The macroscopic activation energy is usually deduced from an Arrhenius-plot based on transport data, such as diffusion coefficient or conductivity. On the microscopic level, ion movement is determined by the individual energy barriers encountered during migration. In heavily doped materials, the corresponding energie landscape is non-uniform, leading to various local barriers due to interactions between charge carriers and point defects such as dopants. As a result, the measured activation energy represents a weighted average of the migration barriers. However, the relationship between the microscopic energy landscape and the macroscopic activation energy remains unknown.

In this contribution, this relationship is explored by applying Kinetic Monte Carlo simulations for various test models. These simulations allow direct control over interaction parameters and thus the energy landscape experienced by charge carriers. This enables the systematic variation of the migration barriers and comparison with resulting activation energies. The simulations reveal that the activation energy itself is temperature-dependent and exhibits complex behaviour even, for model systems. Consequently, reported activation energies from experiments or simulations depend on the corresponding temperature range, and simple models to describe the activation energy often prove inaccurate.