Kinetics of Polaron Capture by Traps in a Lithium Niobate Crystal

Fedorenko Stanislav[1*]

[1] *Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Institutskaya 3, 630090, Novosibirsk, Russia*

** E-mail: fedorenk@kinetics.nsc.ru*

The small-polaron transport plays a key role in the formation of remarkable properties of Lithium Niobate crystals (LN), so attractive for practical applications. Modern time-resolved light induced absorption spectroscopy experiments make it possible to observe the relaxation kinetics of polaron population over a wide range of times [1]. However, the interpretation of experimental data from a microscopic point of view is very difficult due to the complexity of the mechanism of interaction of various types of charge carriers and their capture on traps. Phenomenological analysis of kinetics with the help of widely used Kohlrausch-William-Watts stretched exponential functions does not give anything new in physical understanding [2]. Monte Carlo simulation, unfortunately, does not provide an answer about the microscopic detailing of the kinetic mechanism of polaron capture into traps, without which it is impossible to understand the general kinetic patterns of the process [3].

To correct the situation, we solve the problem of determining the kinetics of polaron relaxation starting from a microscopic description of the polaron dynamics by means of stochastic jumps given by the Markus-Holstein non-adiabatic probability. We focus on the case of Fe doping in LN, when all photo-induced charges are generated from Fe^{2+} centers, which makes it possible to exclude hole polarons from consideration. In this formulation of the problem, three active players remain in the system: free and bound polarons, which can reversibly transform into each other, and Fe^{3+} traps, on which both types of polarons are irreversibly captured.

We have solved this problem analytically. Explicit dependences of the kinetics of free and bound polarons on the microscopic interaction parameters, temperature, and concentration of impurity sites and vacancies are obtained.

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