



Spectral induced polarization in a sandy medium containing semiconductor materials: study of the polarization mechanism

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Preface

The polarization mechanism in mineralized medium is not completely understood yet.

Diffusion of charge carriers inside the semi-conductor grain or around it in the electrolyte: which one is determinant?

The basic equation is not valid in mineralized medium:

$$\tau = \frac{a^2}{D}$$

(after Gurin et al.2015; Revil et al. 2015)

Objectives

New experimental study of the polarization phenomena in mineralized medium (semi-conductors).

New numerical modelling based on Poisson-Nernst-Planck equations has been applied.

Background

Wong (1979) attributes the polarization observed over mineralized medium to two mechanisms:

1- Redox-active ions at the grain surface.

2- Flow of inactive ion in the solution.

- Revil et al. (2015 a, b) attribute the polarization in presence of semi-conductor minerals to the diffusion and accumulation of charges (electrons and holes) inside the metallic grains (in absence of redox activity).
- Both studies show that the metal grain behaves like isolator at lower frequency.

Experiments setup

- Measurements: Complex resistivity of uncosolidated sandy medium
 Variables:
 - 1- semi-conductor content.
 - 2- electrolyte type and concentration (0.001 to 0.5 mol/l).
 - 3- semi-conductor type (galena, pyrite, chalcopyrite and graphite).
 - 4- grain size.
- Background medium
 - Fine grain sand (negligible polarization)
 - Full saturated medium
- Assumption
 - no oxidization.



Calculated parameters

$$\Box \text{ Chargeability:} \qquad M = \frac{\rho_0 - \rho_\infty}{\rho_0}$$

 ρ_0 and ρ_∞ are amplitude of the complex resistivity at lower and higher frequency.

□ The relaxation time:
$$\tau = \frac{1}{2\pi f_{peak}}$$

 f_{peak} is the critical frequency (the frequency of the phase peak).

Semi-conductor content

Example: measurements on Galena of 0.5 mm grain size.



 \checkmark Linear relationship between (*M*) and the volume content semi-conductor.

Electrolyte concentration vs chargeability



 \checkmark No relation between *M* and the electrolyte type or concentration.

Electrolyte concentration vs relaxation time

Example: measurements on 1% volume of Graphite with 10-15 mm grain size.



- ✓ Linear relationship between (τ) and solution conductivity (σ_w).
- ✓ No change in the phase shape and phase amplitude.

Electrolyte type vs mineral type



Semi-conductor grain size



- ✓ Log log relationship between (τ) and a^2 .
- ✓ Negligible change of (τ) with mineral type (Galena and Chalcopyrite).

Modelling assumptions

Poisson-Nernst-Planck equations (PNP):

$$\begin{cases} \frac{\partial c_{i}}{\partial t} = \nabla \left(D_{i} \nabla c_{i} + \frac{z_{i} e}{k_{B} T} c_{i} \nabla V \right); & i = 1, \dots, N \\ \nabla \left(\epsilon \nabla V \right) + \sum_{i} z_{i} e c_{i} = 0 \end{cases}$$

- ❑ This couple of equations describe the influence of the ionic concentration and the electrical potential on the flux of charge-carriers in the medium.
- □ The PNP equations have been applied to model the electromigration diffusion of charge carriers in electrolyte and in semi-conductors.

Numerical calculation

□ The time dependent problem solved by using the finite difference approximation in time (Euler's method).

The space dependent problem solved by using the finite element method.

□ **Freefem++** software is used to perform the numerical computation. (<u>http://www.freefem.org/</u>).



Dirichlet condition = $+V_0/2$

Results of numerical calculation

- □ Assumptions:
- 1- Before injection:
- Potential is zero everywhere in medium
- Homogeneous ions concentration.
- 2- After injection:
- When the particle at center: its own potential is zero all time. (simplification)

Potential distribution



Changing the concentration-Numerically



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Changing the concentration



Correlation in the relation between with the measurements

Qualitative Comparison (Numerical vs experimental)

Measurements and modelling in presence of KCI electrolyte.



Conclusions

- \checkmark *M* is a function of the metal volume and independent of the electrolyte type and concentration.
- \checkmark τ is a function to grain radius, electrolyte conductivity, and slightly to mineral type.
- ✓ The electric dipole formed inside the semi-conductor induces a diffusion of charge carriers in its vicinity.

- ✓ At lower frequency the numerical calculation shows that the grain behaves as isolator.
- ✓ Numerical calculations is in agreement with experimental results and shows a dependence of relaxation time on the electrolyte concentration.

THANK YOU FOR YOU ATTENTION

Outlook

- ✓ Improvement of the numerical model
- ✓ Make computation in frequency domain.
- ✓ Managing the FreeFem++ up scaling to reach more realistic simulation
- ✓ Managing a semi-empiricale model the same as the model of realistic parameters.