Simulation of electron interactions with liquid water and processes related to sub-nanosecond electrical breakdown

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Introduction

Sub-nanosecond electrical breakdown in dielectric liquids is of vital interest, e.g. for applications in high-voltage insulation and high-current switching. Liquid dielectrics in strong nonuniform electric fields are under influence of electrostrictive force that tends to move the fluid into the regions with higher electric field. If the voltage rise is fast enough, the liquid does not have enough time to be set into motion in order to reduce the internal stress. In this case the ponderomotive force induces significant stress in the bulk of the liquid which is manifested as a negative pressure. At certain threshold, the negative pressure causes cavitation ruptures of the fluid. Subsequently, free electrons can be produced by emission from the surface inside the cavity and accelerated to energies exceeding the energy for ionization of water and contribute to ultrafast electrical breakdown of water.

Model description

In this work we investigate conditions under which appearing cavitation nanopores will expand and we will determine their size at the end of the fast voltage pulse, in order to get an estimation of energy that can an electron gain being accelerated in the void [1, 2, 3].

We assume a spherical electrode of radius $r_0 = 100\,\mu$m and voltage amplitude $U_0 = 54\,$kV applied to it in such a way that electric field has a linear ramp with front time t_0:

$$E(r,t) = \frac{U_0 r_0}{r^2} \frac{t}{t_0}. \tag{1}$$

For rapid rise of voltage,for example $t = t_0 = 3\,$ns, the liquid does not have enough time to move and only small changes in hydrostatic pressure are induced. As a result hydrostatic pressure cannot compensate the electrostrictive force and so microcavities are being formed in the closed vicinity of the electrode, where the electrostatic fields is the strongest.

Forces averaged over the surface of microcavity give rise to pressure which consists of

$$P_{\text{av}} = (3/4)(\alpha - 1)\varepsilon_0 \varepsilon E^2 - k_\sigma \sigma / R - p, \tag{2}$$

where the first term represents electrostrictive force, the second corresponds to the surface tension and p is the hydrostatic pressure. Micropores will collapse if $P_{\text{av}} < 0$, on the other hand, if $P_{\text{av}} > 0$, they will expand. Note that electrostrictive pressure will be dominant when compared to hydrostatic pressure p. This will be valid only for fast rise time of the voltage.

Dynamics of the expanding/collapsing microcavity given by the balance for the kinetic energy of expanding fluid and by the work of pressure forces. We obtain equation for development of microcavity radius $R(t)$:

$$\frac{d}{dt}\left(R^3\left(\frac{dR}{dt}\right)^2\right) = \frac{4}{\rho}R\frac{dR}{dt}\left(\frac{3}{8}R(\alpha - 1)\varepsilon_0 \varepsilon E^2 - \frac{pR}{2} - k_\sigma \sigma\right). \tag{3}$$

Then using (1) and introducing variables $x = (R/R_0)^{5/2}$, where R_0 is the initial size of the microcavity, and $\tau = t/t_0$, and substituting

$$\tilde{P}_{max} = \frac{(\alpha - 1)\varepsilon_0 \varepsilon}{2}\left(\frac{U_0}{r_0}\right)^2,$$

the equation (3) can be written in a form:

$$\frac{d^2 x}{dt^2} = 5\frac{\sigma t_0^2}{\rho R_0^3}x^{-1/5}\left[\left(\frac{3\tilde{P}_{\text{max}}R_0}{4\sigma}\left(\frac{r_0}{r}\right)^4 \tau^2 - \frac{pR_0}{2\sigma}\right)x^{2/5} - k_\sigma\right]. \tag{4}$$

It follows that micropore starts to expands at

$$\tau_0 = \frac{(pR_0/(2\sigma) + k_\alpha)}{\sqrt{3\tilde{P}_{max}R_0(r_0/r)^4/(4\sigma)}},$$

and the expansion region is limited to

$$\frac{r}{r_0} < \left(\frac{3\tilde{P}_{max}R_0}{4\sigma(k_\alpha + pR_0/(2\sigma))}\right)^{1/4}.$$

In the following we present numerical solution of (4) for parameters: $r_0 = 100\,\mu\text{m}$, $\varepsilon = 81$, $\alpha = 1.5$, $U_0 = 54\,\text{kV}$, $t_0 = 3\,\text{ns}$, $\sigma = 0.072\,\text{N/m}$, $R_0 = 2\,\text{nm}$, and $k_\alpha = 1$. We also assume that electrostrictive pressure is much stronger than hydrostatic pressure, so that $p \approx 0$.

Figure 1a shows the radius of expanded micropore as a function of distance from the electrode at the end of the voltage rise time. Figure 1b shows possible energy gain of an electron crossing the cavity diameter as a function of distance from the electrode at the end of the voltage rise time. Vertical lines separates regions, where ionization of water is and is not possible. It's clear

that at given conditions, ionization of water molecules is possible only in the near vicinity of the electrode.

Model for expansion of micropores allows to find time dependence of microcavity radius at the end of the voltage rise time and determine energy that electron can gain inside the cavity as a function of distance from the electrode. Thus we are able to identify volume in the vicinity of the electrode where ionization of water through the cavity mechanism is possible.

Having geometrical parameters of ionization region enables us to investigate electrical break-down on the microscopic scale using Monte-Carlo collision models. For this purpose Geant4-DNA [9, 10] seems to be one of the best available tools. Using Geant4-DNA we simulated development of electron avalanche originating from one electron accelerated on the set of cavity/liquid water layers, see the figure 2.
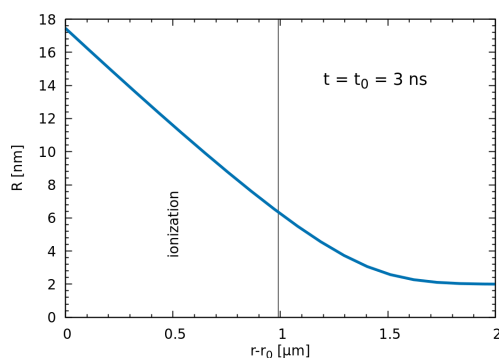
(a) *Radius of expanded micropore as a function of distance from the electrode at the end of the voltage rise time. Vertical line separates regions where ionization of water is and is not possible.*
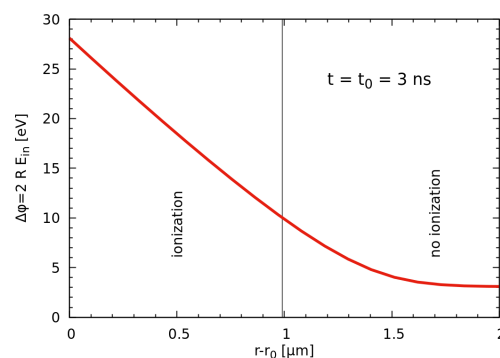
(b) *Energy gained by an electron crossing the cavity as a function of distance from the electrode at the end of the voltage rise time. $E_{in} = 3\varepsilon E/(1+2\varepsilon)$, with E given by eq. (1) for $t = t_0$ [3]. Vertical line separates regions where ionization of water is and is not possible.*

Figure 1: *Development of nanopores in inhomogeneous pulsed electric field.*

Conclusion

Presented model gives basic ingredients necessary to study interaction of accelerated electrons with water. Obvious next step is to determine conditions necessary for electron multiplications and subsequent build up of space charge, we believe that the Geant4-DNA could be an appropriate tool to do this. Space charge then serves as an virtual electrode and cavitation and ionization of water can, under certain condition proceed further form the electrode, following
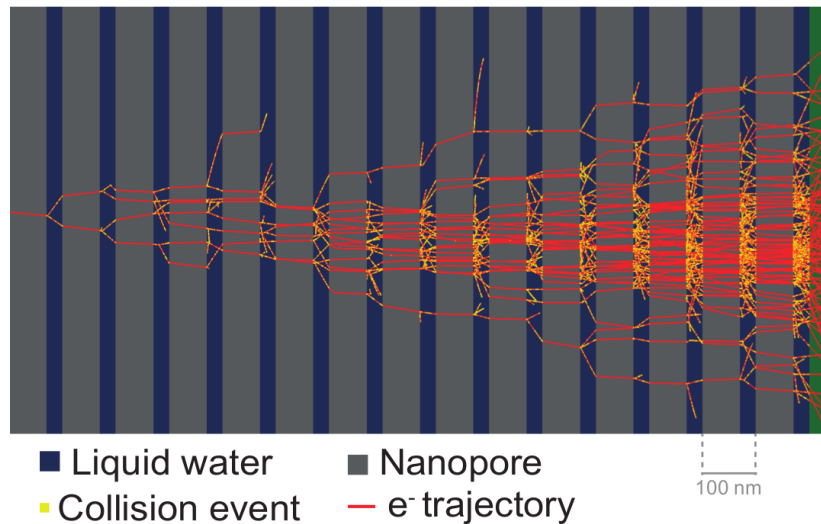
Figure 2: *Electron avalanche simulated using program Geant4-DNA.*

the same mechanism of micropore expansion in high electric fields.

Acknowledgement

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