Temperature Effect to the Dissolution and Deposition of Dental Metallic Biomaterials-A Theoretical Model in Cyclic Voltammetry

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Abstract: In this work, we present an on-line MATHCAD protocol that allows calculation of cyclic voltammograms related to dissolution and deposition of dental metallic biomaterials at different temperatures. The model provides insights on how the temperature affects the processes of dissolution/deposition via the cyclic voltammograms of the metallic dental biomaterials. While we present plenty of calculated cyclic voltammograms at different temperatures, we also give hints how the kinetics of dissolution/deposition process of metallic dental biomaterials can be evaluated from the features of simulated voltammograms

$tac := 0.01$

$Es := -0.4 \quad Ef := 0.4 \quad \Delta E := Ef - Es \quad dE := 0.004 \qquad \tau := 0.01 \quad d := \frac{\tau}{25}$

$m := \frac{tac}{d} + 1 .. \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} \qquad n := \frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d} + 1 .. \left(\frac{\Delta E}{dE} \cdot 25 \cdot 2 + \frac{tac}{d}\right)$

$i := 1 .. \frac{tac}{d}$

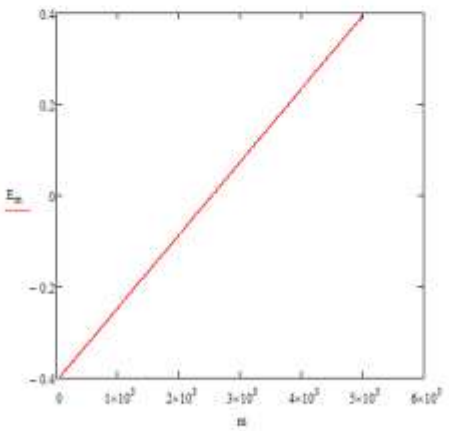
$\frac{\Delta E}{dE} = 200$

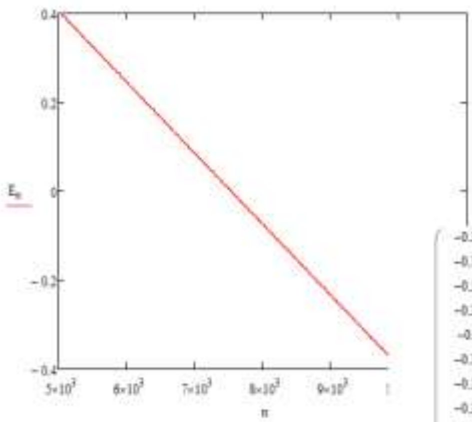
$E_m := Es + \left(ceil\left(\frac{m - \frac{tac}{d}}{25}\right) \cdot dE - dE\right)$

$E_n := Ef - \left[ceil\left[\frac{n - \left(\frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d}\right)}{25}\right] \cdot dE - dE\right]$

$\frac{dE}{\tau} = 0.4$

ECrev Mechsnism of Metallic Dissolution/Deposition
Red(ads) -1e- = Ox(dissolved)
in Cyclic Voltammetry
IF Equilibrium Constan M > 100, mechanism converges to simple Red(ads) -1e = OX(dissolved)
Mechanism
K is dimensionless kinetic parameter related to electrde reaction
γ is dimensionless catalytic parameter related to follow up chemical reaction
α is electron transfer coefficient
M is equilibrium constant of follow up chemical reaction
kf and kb are forward and backward rate constants of folow up chemical reaction
Es is starting potential
Ef is final potential
dE is potential step
Ψ is symbol for dimensionless current
Em is cathodic potential ramp in cyclic voltammetry
En is anodic potential ramp
Sk is integration factor
τ is duration of potential steps
D is diffusion coefficient of Ox





−0.396
−0.392
−0.388
−0.384
−0.38
−0.376
−0.372
−0.368
−0.364
−0.36
−0.356
−0.352
−0.348
−0.344
−0.34
−0.336
−0.332
−0.328
−0.324
−0.32
−0.316
−0.312
−0.308
−0.304
−0.3
−0.296
−0.292
−0.288
−0.284
−0.28
−0.276
−0.272

$A := 0.28 \qquad cox := 0.0000008 \qquad w := 1.000001000062$

$ks := 0.2 \qquad D := 3 \cdot 10^{-8} \qquad kf := .000222210 \qquad 0.05 \quad \varepsilon$

$K := \frac{ks \cdot \sqrt{\tau}}{\sqrt{D}} \qquad \alpha := 0.5 \qquad kb := .00022225010 \qquad 0.075$

0.35

$M := \frac{kf}{kb}$ Konstanta na ramnoteza

$\log(K) = 1.062 \quad K$

$M := 22222.1000$

$F := 96500 \quad el := 2 \quad R := 8.314 \quad T := 298.15$

$\varepsilon := kf + kb$ kineticki parametar $\qquad k := 1 .. 2\left(\frac{\Delta E}{dE} \cdot 25 + \frac{tac}{d}\right)$

$\Phi_m := el \cdot \frac{F}{R \cdot T} \cdot (E_m) \quad b_n := el \cdot \frac{F}{R \cdot T} \cdot (E_n)$

$r := \varepsilon \cdot \tau$

$S1_k := \sqrt{\frac{k}{25}} - \sqrt{\frac{k-1}{25}}$

$z := (kf + kb)^{0.5} \cdot \tau$

$z = 2.108 \times 10^{-3}$

-3

$\Phi ac := el \cdot \frac{F}{R \cdot T} \cdot Es$

$\gamma := h \cdot 1$

$\cdot 3$

$\gamma = 2.108 \times 10^{-3}$

$S_k := \left(1 - erfc\left(\sqrt{\frac{\varepsilon \cdot \tau}{25} \cdot k}\right)\right) - \left[1 - erfc\left(\sqrt{\frac{\varepsilon}{...}}\right.\right.$

$$\Phi ac := el \cdot \frac{F}{R \cdot T} \cdot Es$$

$$\gamma := h \cdot 1$$

$$\gamma = 2.108 \times 10^{-3}$$

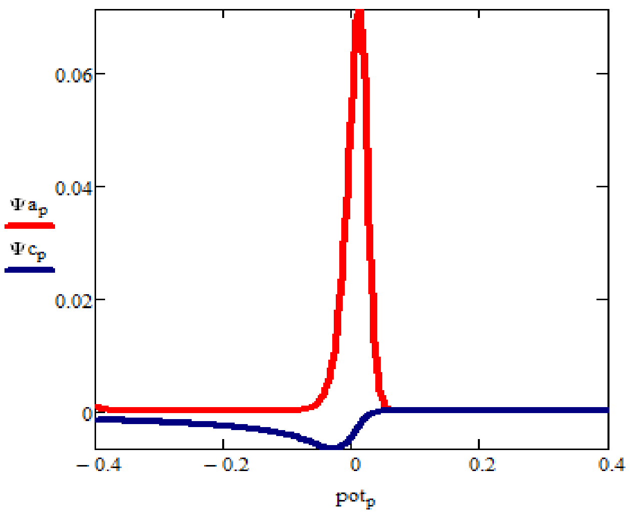
$$\Psi_1 := \frac{K \cdot e^{\alpha \cdot \Phi_1}}{\left[1 + \frac{0.04 \cdot K \cdot e^{(1-\alpha) \cdot \Phi_1} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{1 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi_1}}{\sqrt{\pi \cdot 1}} \cdot \frac{M}{1+M}\right] + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi_1} \cdot S_1}$$

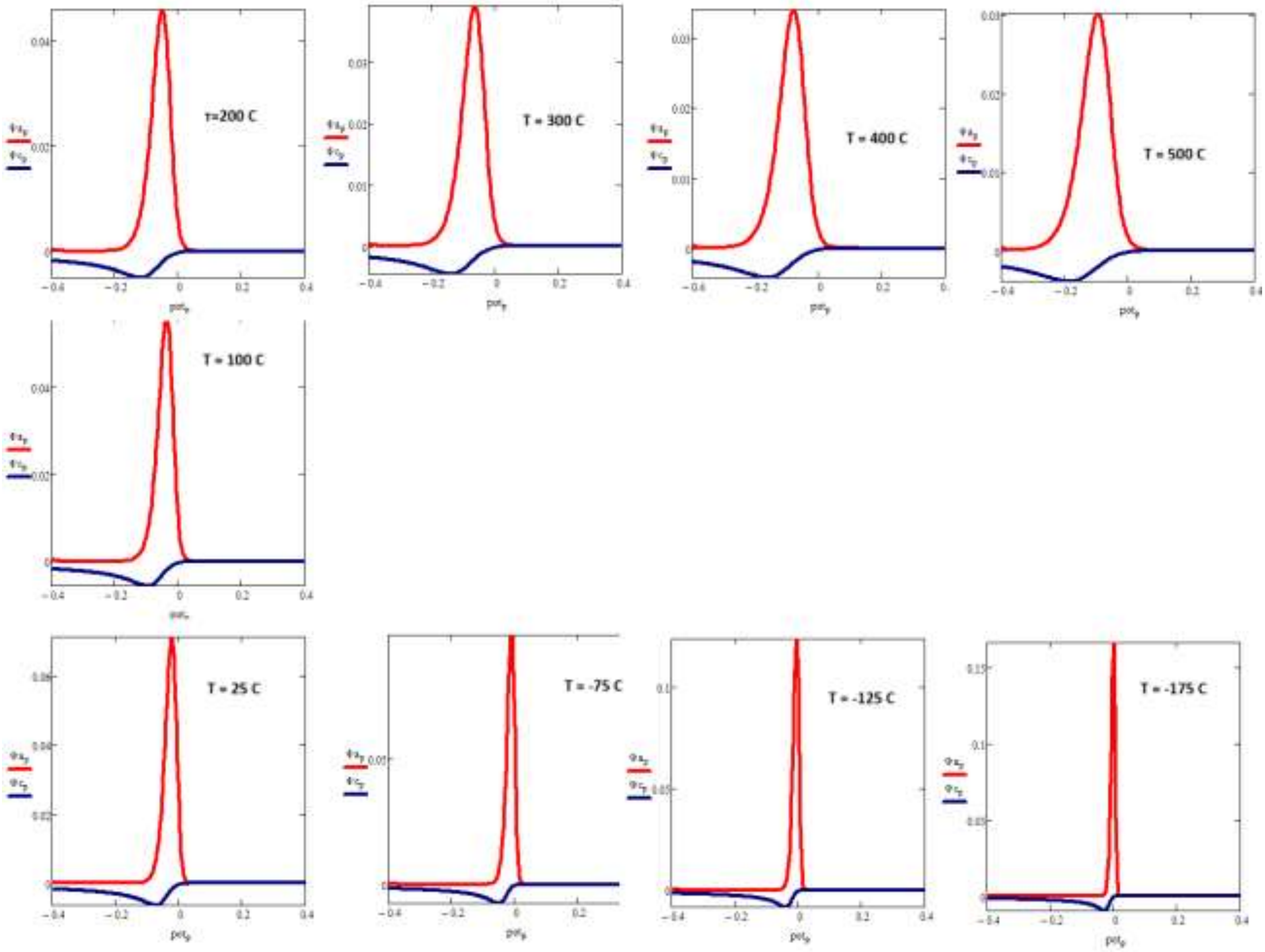
$$\Psi_s := \frac{K \cdot e^{\alpha \cdot \Phi ac} - \frac{0.04 \cdot K \cdot e^{\alpha \cdot \Phi ac}}{\sqrt{1 \cdot 1}} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot 1\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi ac}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S1_{s-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi ac} \cdot \sum_{j=1}^{s-1} \left(\Psi_j \cdot S_{s-j+1}\right)}{1 + \frac{0.04 \cdot K \cdot e^{\alpha \cdot \Phi ac} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi ac}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi ac} \cdot S_1}$$

$$\Psi_m := \frac{w \cdot e^{\alpha \cdot \Phi_m} - \frac{0.04 \cdot w \cdot e^{\alpha \cdot \Phi_m}}{\sqrt{1 \cdot 1}} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot 1\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi_m}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S1_{m-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi_m} \cdot \sum_{j=1}^{m-1} \left(\Psi_j \cdot S_{m-j+1}\right)}{1 + \frac{0.04 \cdot w \cdot e^{\alpha \cdot \Phi_m} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot \Phi_m}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot \Phi_m} \cdot S_1}$$

$$\Psi_n := \frac{w \cdot e^{\alpha \cdot b_n} - \frac{0.04 \cdot w \cdot e^{\alpha \cdot b_n}}{\sqrt{1 \cdot 1}} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot 1\right) - \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot b_n}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S1_{n-j+1}\right) - \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot b_n} \cdot \sum_{j=1}^{n-1} \left(\Psi_j \cdot S_{n-j+1}\right)}{1 + \frac{0.04 \cdot w \cdot e^{\alpha \cdot b_n} \cdot 1}{\sqrt{1 \cdot 1}} + \frac{2 \cdot K \cdot e^{-(1-\alpha) \cdot b_n}}{\sqrt{\pi \cdot 25}} \cdot \frac{M}{1+M} + \frac{\gamma}{1+M} \cdot e^{-(1-\alpha) \cdot b_n} \cdot S_1}$$

$p := 1 .. \frac{\Delta E}{dE}$ $\quad \Psi a_p := (\Psi)_{\left(\frac{\tau}{d \cdot 25} + p\right) \cdot 25}$ $\quad \Psi c_p := (\Psi)_{\left[\left[\frac{\Delta E}{dE} \cdot 2 + \left(\frac{\tau}{25 \cdot d}\right)\right] - p\right] \cdot 25}$ $\quad pot_p := Es + p \cdot dE$





Effect of temperature to the process of dissolution/deposition of dental metallic biomaterials depicted in the features of calculated cyclic voltammograms

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