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Nafion-Based Ionic-Polymer-Metal Composites: Displacement Rate Analysis by Changing Electrode Properties

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ABSTRACT

In this paper, a polymer-metal ion composite is modeled in two dimensions. The core material is Nafion 117 and the electromechanical effects of electrodes with four different materials of aluminum, gold, copper, and titanium on the stress and displacement are investigated by finite element method. Based on the properties of each material such as corrosion resistance, conductivity cost of metals and the results of the analysis, aluminum has the maximum displacement and copper is the most conductive metal but they oxidize quickly in contact of air or water. On the other hand, gold has excellent resistance to erosion and can be manufactured with very thin thickness. It has also been shown that titanium is not an optimal metal due to its scarcity and properties contrary to the needs of an efficient IPMC. Also, the stress created in the piece is almost equal in all four cases.

KEYWORDS IPMC, Displacement, Finite element, Electromechanical, Smart material composite.

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INTRODUCTION

Mechatronics systems are shrinking so that micro, meso and nano-robots will play a wide range role in the near future. The manufacture of these materials requires innovation in manufacturing methods.[1] Also, to achieve this field of science, it is necessary to make smart materials. The most widely used material in the world with electromechanical properties are piezoelectrics.[2] The ion-polymer-metal composite (IPMC) has a much higher displacement than the above-mentioned material. IPMCs are smart materials that consist of ionic polymer sheet like Nafion or Flemion whose surfaces are roughened with noble metal such as gold or platinum as sources of electrodes.[3] Under applying small amount of voltage, the polymer sheet bends significantly.[4] On the other hand, if a deformation is applied to IPMC, it results in generating output voltage.[5] This special behavior can be used in various industries for different applications. For example, they are expected to be used as actuators, sensors, or artificial muscles.[6] Also they play a part in microelectromechanical systems (MEMS) which are technologies to manufacture complex structures and devices within the size range of 1 μm up to 1 mm.[7] In fact, IPMCs are part of a larger group of polymers called EAPs (electroactive polymers) which in respond of electric stimulation, their properties change. IPMC has some different properties and advantages over EPA because not only it's a polymer, but also it's a composite.[4] Some of these properties are small amount of activation voltage, bending deformation, light weight, and flexibility.[8] Moreover, they are difficult to control and produce poor generative force which are its disadvantages among others.[9] Therefore, careful investigating different aspects of IPMCs are crucial for developing novel applications for such materials.

In this research, we propose four different electrode material models in COMSOL Modeling Software and discuss the effects on displacement and stress. These materials are gold, copper, titanium and aluminum and the properties of polymer are presumed constant. Due to different characteristic of materials we also need to take into account other aspects of these metals like Young's modulus, Poisson's ratio, density, relative permittivity, oxidization process, and price. Each of these features has its advantages and disadvantages. For instance, by applying a small voltage, the use of one of the substance may lead to quicker respond in comparison to other substances, but it oxidizes faster in contact with air or aquatic environments. Therefore, the results of this study help to select a suitable IPMC according to its characteristics for the intended application.

MATERIALS & METHODS

Modeling

We modeled a 10 mm long rectangular film strip with a Nafion thickness of 0.07 mm and an electrode thickness of 1 µm on both sides of Nafion. This 2D model is developed by finite element method with approximately 112000 triangle shaped elements. The results were not affected from 112000 triangles onward; therefore, the optimized type of mesh was obtained. Other details of mesh elements are given in Table 1 and the meshing structure is showed in Fig. 1.

Table1: Details of finite elements.

Minimum element quality	0.3907
Average element quality	0.8658
triangle	112774
Edge element	25566
Vertex element	20
Minimum element size	0.5
Maximum element size	3.3
Resolution of narrow regions	0.9
Maximum element growth rate	2
Predefined size	Extremely coarse

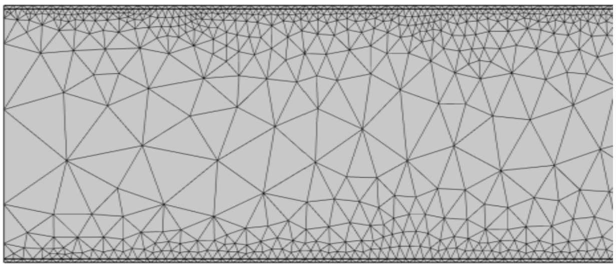

Fig. 1: Meshing illustration.

A simple illustration of IPMC deformation after applying a small voltage is shown in Fig. 2.

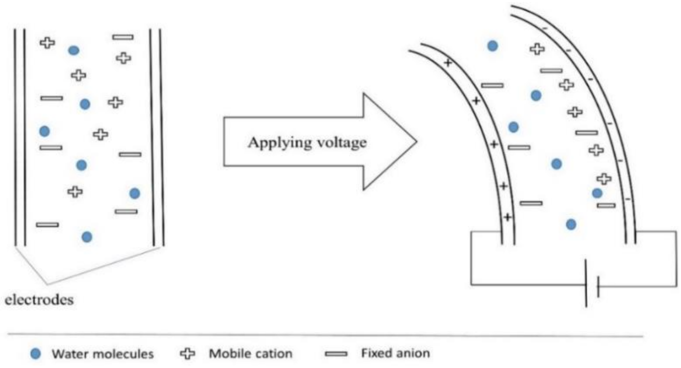

Fig. 2: Illustration of IPMC actuation mechanism.

If σ stands for stress and ρ is electric rate charge, then eq. (1) can be derived.[10]

$$\sigma\ (x, y, z, t) = \alpha_0\rho\ (x, y, z, t) \tag{1}$$

In eq. (1), α_0 is coupling constant calculated experimentally. Using the equations of continuous space, the ion flux vector inside the IPMC transducer is obtained in eq. (2).[11]

$$J = -d\ (\nabla\ C^+ + \frac{C^+ \cdot F}{RT} \nabla\varphi + \frac{C^+ \cdot \Delta v}{RT} \nabla p) + C^+\ v \tag{2}$$

Here d is Ionic diffusivity, C^+ is Cation concentration, F is Faraday constant, R is Ideal gas constant, T is Absolute temperature, φ is electric potential, Δv is volume change, and p is free velocity. Thickness is much smaller than its length and width, therefore; the result can be restricted along the x-axis.

By generalizing the above relation and since the piezoelectricity depends on the vector of J ion changes and cationic concentration C^+, eq. (3) can be derived.[12]

$$\frac{\partial}{\partial x} [\ \partial \frac{(kF)}{\partial t} - d \frac{\partial^2 (kE)}{\partial x^2} + \frac{F^2\, dC}{kRT} - (1 - C^- \cdot \Delta v)(kE)\ ] = 0 \tag{3}$$

C^- is anionic concentration and k is the effective dielectric constant of the polymer. The answers of eqs. (2) and (3) are examined below.

First of all, it should be noted that IPMC material is composed of two outer layers of noble metal as electrode, polymer ion membrane with fixed anions and moving cations on both sides. Due to the presence of fixed anion layers, the voltage step used leads to asymmetric ion distribution, which is neglected.

Considering the solution of the implicit equation under the conditions of asymmetric ionization of ions, we solve the equation.[13] Considering the stability condition $j = 0$ and $\left(\frac{\partial c^+}{\partial x}\right) = 0$, eqs. (2) and (3) are written as eq. (4).[13]

$$\frac{\partial^2 E}{\partial x^2} - kE = 0 \ \text{ and } \ k = \frac{F^2 C^-}{kRT}(1 - C^- \Delta v) \tag{4}$$

Note that the charge density is examined in two separate areas. In the anodic boundary layer, the charge density is constant and is shown as $\rho(1) = -C^- F$ and in the rest we have, $\rho(2) = (C^+ - C^-)F$. The charge density (ρ), electric field (E) and electric potential (ϕ) in the anodic boundary layer are given in eq. (5).[14]

$$\begin{aligned} &\rho(1)^{(x)} = -\ C^- F \\ &E(1)^{(X)} = \frac{1}{K} (-\ C^- F_X + E_0\ ),\ (-h \leq x \leq -h +\ w) \\ &\phi(1)^{(X)} = \frac{1}{K} (\frac{C^-\ F_X^2}{2} - E_{0\,x}\ ) + A_0 \end{aligned} \tag{5}$$

Integrating eq. (5) according to the dynamics of a charging model is described in eq. (6).[11]

$$(x, t) = (1 - exp\,(-t/\ \tau))\ \rho * (x)\ ,\ \tau = \frac{kRT}{dC - F} \tag{6}$$

Here, τ is the time required to charge the cations. Due to the load density scatter, we can measure the amount of internal stress σ in an IPMC actuator by applying a voltage ϕ. The amount of stress σ varies along the thickness of the IPMC actuator but along the plane x-y remains constant.

Internal stress σ causes a deformation wave in the IPMC actuator. To simplify the analysis, we use a visual modeling method using the Multiphysics Comsol and the finite element method for IPMC stimulus modeling. The internal stress σ, obtained from eq. (1), is added to the finite element to investigate the deformation. The constraints on the involved edges of the IPMC actuator are then considered as boundary conditions, and the deformation limit is applied to the neutral plate inside the actuator.

For describing our work, it is noted that one side of the beam is fixed, which means we have zero displacement according to eq. (7).[15]

$$u = 0 \tag{7}$$

By applying constant voltage of 5 V, the amount of stress and displacement during the actuator is obtained. Fig. 3 shows the deformation of the IPMC with a fixed voltage 5 V and aluminum electrodes.

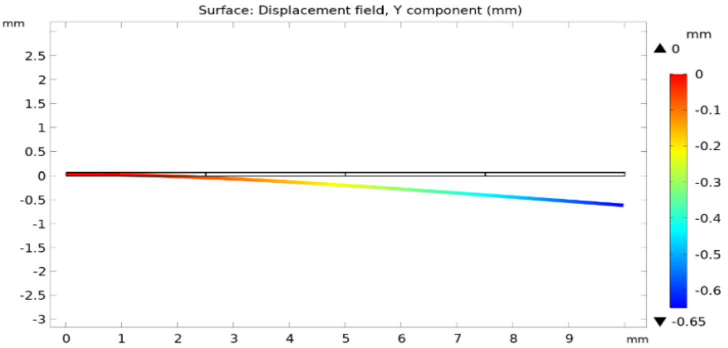

Fig. 3: Deformation of the piece in the direction of the *y*-axis.

Nafion

Table 2 shows properties of polymer part of IPMC. Note that in this analysis, the properties of core (Nafion) are constant.

Table 2: Properties of Nafion.[16]

Property	Variable	Value	Unit
Density	ρ	3385	kg/m^3
Poisson's Ratio	*nu*	0.487	1
Young's Modulus	*E*	0.5e9	*Pa*
Relative Permittivity	*epsilon*	1	1

Aluminum

Ingredients, manufacturing processes and heat treatment change the properties of materials.[17] Aluminum is a light and ductile metal with high mechanical strength which can be improved by adding alloying elements. Pure aluminum has low electric resistivity, therefore, according to eq. (2), it has high electric conductivity as indicated by eq. (8).[18]

$$G = 1/R \tag{8}$$

In eq. (8), G stands for electric conductivity and R shows electric resistivity. When exposed to oxygen, aluminum forms a protective layer of aluminum oxide (Al_2O_3), which protects the metal from corrosion and rust. This layer reduces electric conductivity and strengthens mechanical properties.[18] Some of aluminum properties are mentioned in Table 3.

Table 3: Properties of aluminum.

Property	Variable	Value	Unit
density	ρ	2730	kg/m^3
Poisson's ratio	*nu*	0.33	1
Young's modulus	*E*	69e9	*Pa*
Relative permittivity	*epsilon*	1	1

Copper

Copper is a very malleable metal and is one of the lowest metals in terms of electrical resistance. This makes it the second most conductive metal among others. It resists oxidation at room temperature but oxidizes at higher temperatures. However, it does not oxidize in aqueous media.[19] Some of the copper constant values are pointed out in Table 4.

Table 4: Properties of copper.

Property	Variable	Value	Unit
density	ρ	8960	kg/m^3
Poisson's ratio	*nu*	0.35	1
Young's modulus	*E*	110e9	*Pa*
Relative permittivity	*epsilon*	1	1

Gold

As presented in Table 5, gold is the most malleable and ductile metal with high density. Hence, it can be manufacture in layers of gold with a very small number of atoms and form very thin sheets. Gold has a fine corrosion resistance and a good electric conductivity. Despite all of the useful properties of gold, it's still one of the most expensive metal in the world.[20]

Table 5: Properties of copper.

Property	Variable	Value	Unit
density	ρ	19300	kg/m^3
Poisson's ratio	*nu*	0.44	1
Young's modulus	E	70e9	*Pa*
Relative permittivity	*epsilon*	1	1

Titanium

Titanium properties are a combination of high strength and low density. It shows high corrosion resistance at different range of temperatures. Titanium is not a good conductor of electricity because it has a very high electric resistivity. Titanium powder is more difficult to prepare and when it comes to purchasing, it's a rare metal.[21] Table 6 shows some constant values of titanium that has been used in finite element analysis.

Table 6: Properties of titanium.

Property	Variable	Value	Unit
density	ρ	4506	kg/m^3
Poisson's ratio	*nu*	0.321	1
Young's modulus	E	115.7e9	*Pa*
Relative permittivity	*epsilon*	1	1

RESULTS & DISCUSSION

Fig. 4 shows the displacement changes with the aluminum electrode, with a maximum amount of 650 micrometers and Fig. 5 is its von Misses stress.

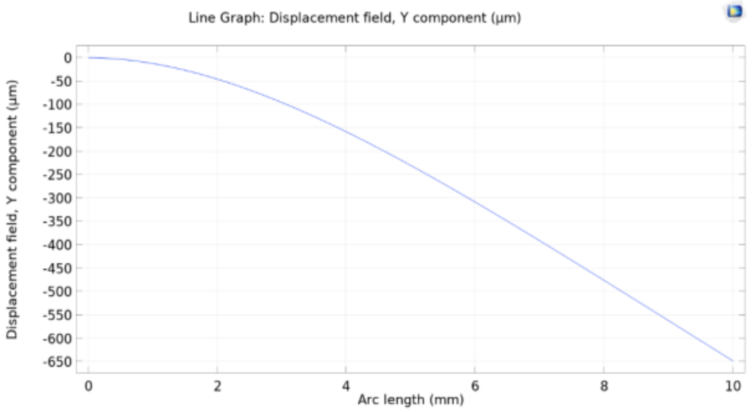

Fig. 4: Displacement of IPMC with aluminum electrodes.

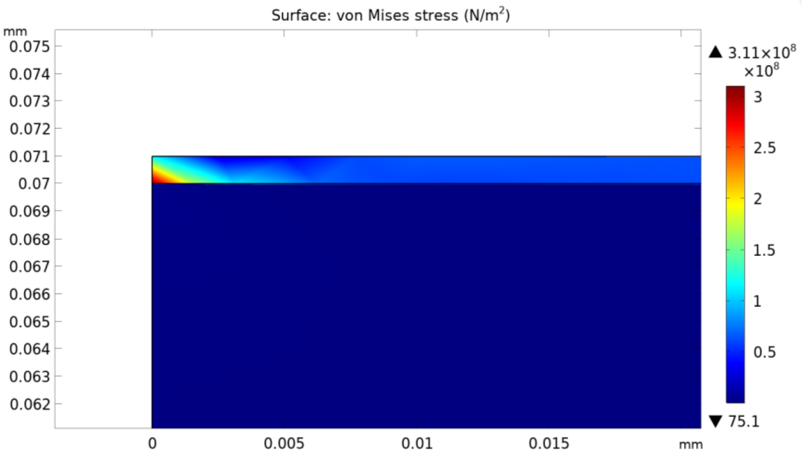

Fig. 5: von Mises stress of IPMC with aluminum electrodes.

Displacement of copper model is plotted in Fig. 6 with maximum amount of 430 micrometers or thereabout and maximum stress of copper is 3.29×10^8 (N/m^2) as shown in Fig. 7.

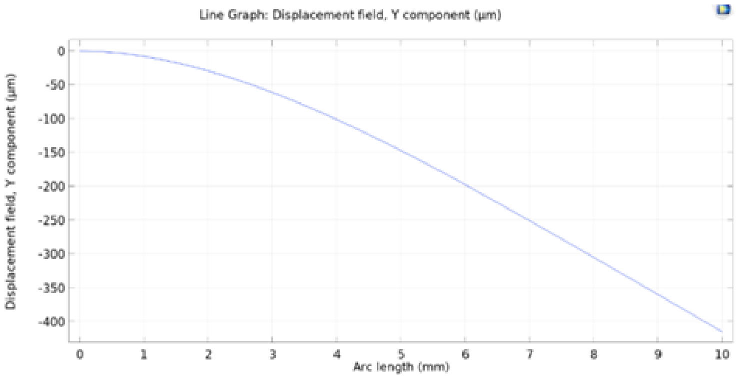

Fig. 6: Displacement of IPMC with copper electrodes.

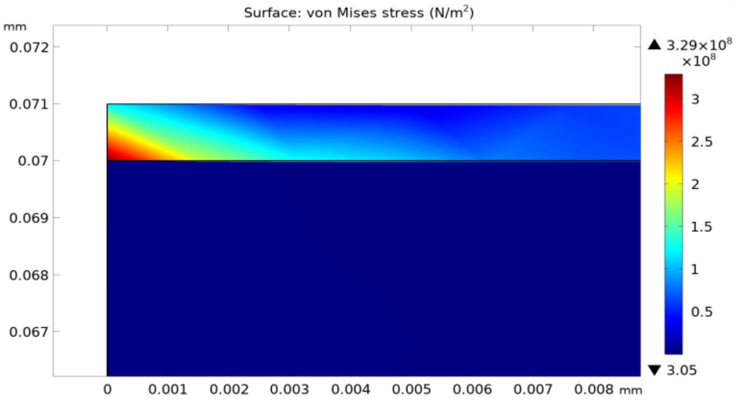

Fig. 7: von Mises stress of IPMC with copper electrodes.

For electrodes with gold material, Fig. 8 and Fig. 9 are respectively displacement diagram and stress analysis. The peak of displacement is approximately 550 µm and max stress is 3.16×10^8 (N/m^2).

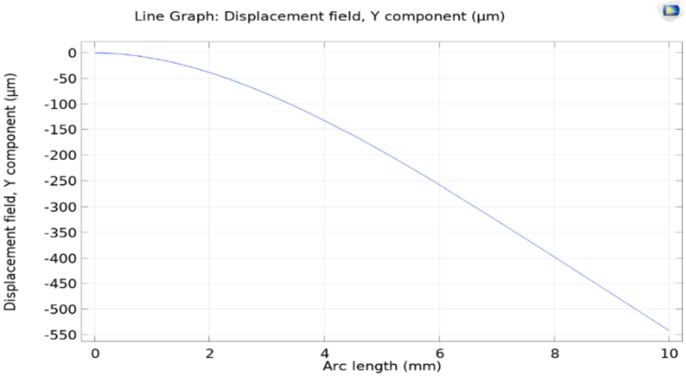

Fig. 8: Displacement of IPMC with gold electrodes.

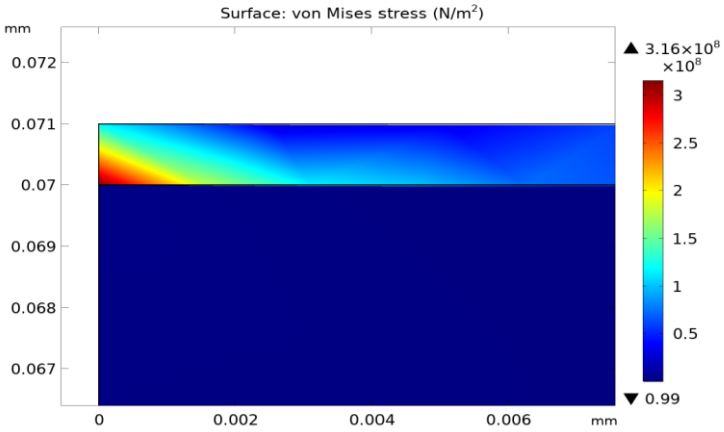

Fig. 9: von Mises stress of IPMC with gold electrodes.

At last but not the least, with titanium electrodes the maximum absolute value of displacement is about 410 micrometers and the max stress is 3.32×108 (N/m^2), which are presented in Fig. 10 and Fig. 11.

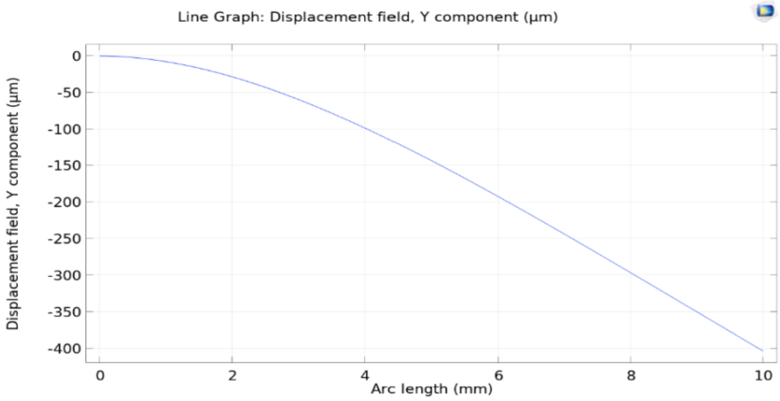

Fig. 10: Displacement of IPMC with titanium electrodes.

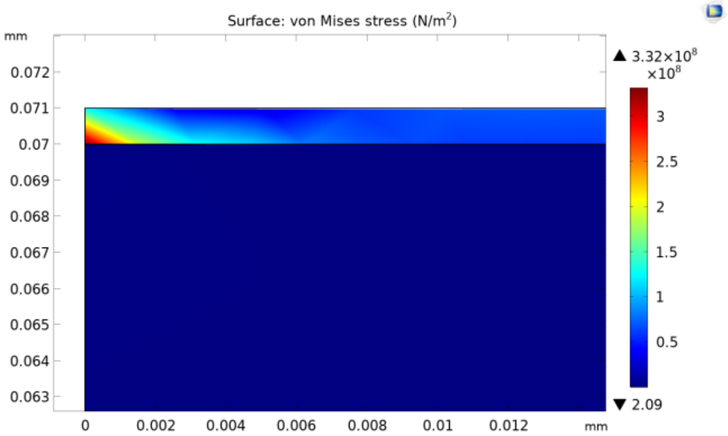

Fig. 11: von Mises stress of IPMC with titanium electrodes.

According to what has been presented so far, aluminum has the highest displacement, lowest price and is in second place in conductivity. However, due to its fast oxidization in contact of air, a hard layer of aluminum oxide is formed on the surface which makes the movement of the actuator difficult. It also reduces the longevity. The second in displacement is gold with almost zero oxidation and acceptable conductivity but it is the most expensive one. Gold can be a proper material for electrodes because it can be very thin on a micro scale. The results show that although copper has lower movement than aluminum or gold, but it is the most conductive metal with affordable price. However, it has low corrosion resistance. In the case of titanium, it has the bottommost conductivity and displacement. Moreover, it is an expensive and a rare metal; hence, it's not a suitable material.

CONCLUSION

In summary, the IPMC composite in the form of a single beam with four different electrodes of aluminum, gold, titanium and copper has been modeled. By applying a voltage of 5 volts, the stresses created as well as the total displacement of the part have been investigated by finite element method and the relevant diagrams have been drawn. Displacement changes in order from large to small are for aluminum, gold, copper, and titanium. Also the results have been compared to conductivity, oxidation, and price of the materials. Gold, in compare of other metals, has more suitable properties with acceptable displacement which make it a qualified metal for electrodes.

DISCLOSURE STATEMENT

The author(s) did not report any potential conflict of interest.

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