

# THEORETICAL MODEL AND FINITE ELEMENT SIMULATION OF THE EFFECTIVE ELECTROMECHANICAL PROPERTIES OF CELLULAR PIEZOELECTRET FILM

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**Summary** By taking the voids containing electric charges of opposite polarities as ellipsoidal piezoelectric inclusions and the polymer as matrix, we presented a micromechanical model for the effective electromechanical properties of cellular piezoelectret film. Qualitative analysis and quantitative comparison with experiments verify the validity of the model. Furthermore, we developed a finite element model to simulate the effective piezoelectric coefficient of cellular piezoelectret film. The disk-shaped microvoids are modeled geometrically by the three-dimensional hollow oblate tetrakaidecahedra. The polymer is taken to be isotropic and viscoelastic. Temporal evolution of the effective piezoelectric  $d_{33}$  coefficient in the film thickness of cellular piezoelectret film can be obtained.

## MICROMECHANICAL MODEL FOR THE EFFECTIVE PROPERTIES OF CELLULAR PIEZOELECTRET FILM

Cellular piezoelectret film is actually voided charged polymer film. When the polymer pre-mixed with mineral particles is biaxially stretched to a thin film, a large number of closed flat microvoids can be produced. Under high electric field, internal breakdown occurs to the air inside microvoids. Electric charges of opposite polarities deposit on the upper and bottom parts of the internal surfaces of voids. The disk-shaped microvoids with trapped electric charges behave like giant dipoles. Macroscopically, the voided charged polymer film shows highly sensitive quasi-piezoelectric effect in the film thickness direction. Together with the flexibility, cost effectiveness in preparation, low acoustic impedance matched to water and human body, cellular piezoelectret film shows great potential in application such as medical diagnostics, nondestructive testing and other sensor technology [1-3].

Experiments demonstrate that the overall properties of cellular piezoelectret film are closely related to the void microstructures. For example, controlled inflation of cellular piezoelectret film considerably changes the effective electromechanical properties in the film thickness direction [4, 5]. It is expected that optimization can be conducted to find the largest piezoelectric  $d_{33}$  coefficients by regulating the void shape and void fraction. Theoretical models are required. The sandwich model [6, 7] of solid layers and air layers has been frequently quoted in literature for theoretical simulation of cellular piezoelectret film. This model is too simplified to explicitly uncover the basic mechanism of electromechanical coupling and microstructures. Haberman et al [8] presented a more sophisticated three-dimensional model, but still lack quantitative comparison between theoretical and experimental results. We have developed a micromechanical model to find the effective electromechanical moduli of cellular piezoelectret film. We treat cellular piezoelectret film as piezoelectric composite. The polymer is taken as the dielectric matrix, without piezoelectricity but with permittivity, and the voids with distributed charges as ellipsoidal inclusions, which can be endowed with a piezoelectric coefficient [9,10]. The effective moduli can be found by extending into electromechanical coupling the classical Equivalent Inclusion Method and the differential scheme. Qualitative analysis with respect to various material parameters and void geometric variables for the predicted overall electromechanical behavior shows consistency with experimental observation. Quantitative comparison with the inflation experiments was also conducted, as shown in Fig. 1 and Fig. 2, where the abscissa denotes the relative density and the vertical coordinate is, respectively, the elastic modulus and piezoelectric coefficient in the thickness direction. The solid dots represent the experimental results in [4]. General agreement can be achieved for the theoretical and experimental results.

## FINITE ELEMENT SIMULATION FOR THE TEMPORAL EVOLUTION OF THE EFFECTIVE PROPERTIES OF CELLULAR PIEZOELECTRET FILM

Since polymer is generally viscoelastic, the effective properties of cellular piezoelectret film usually show time-dependent behavior [10,11]. We have developed a finite element model to simulate temporal evolution of the effective quasi-piezoelectric  $d_{33}$  coefficient of cellular piezoelectret film. Under external electric field, the electric charges trapped on the internal surfaces of voids are subjected to electrostatic forces which are directly transferred onto the host polymer. The elastic deformation occurs and the piezoelectric  $d_{33}$  coefficient can be phenomenologically defined. Film thickness variation is calculated when a voltage difference is applied on the piezoelectret film. This can be accomplished by solving the elastic deformation under the electric-field-induced forces provided by the Maxwell stress tensor. For the finite element geometric model, since the microvoids in cellular piezoelectret film generally have the almost same size in two orthogonal in-plane directions and a much smaller thickness in the out-of-plane direction, we propose that the cellular piezoelectret film be modeled as the periodic composite, and the closed disk-shaped microvoids be modeled by the three-dimensional hollow oblate tetrakaidecahedra, which is actually composed of two nested tetrakaidecahedra [12]. We select the Representative Volume Element (RVE) as the smallest repetitive cuboid

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that compactly encloses the outer tetrakaidecahedron. The Solid226 coupled-field hexahedron element with 20 nodes in ANSYS<sup>®</sup> is used to mesh the RVE. Periodic boundary conditions are imposed. The elastic displacement is kept to zero in the normal direction of the four side planes. The bottom plane is completely constrained and the top plane is mechanically free. As for the electrical boundary conditions, the normal electric displacement vanishes on the four side planes, while the electric potential is kept to zero on the bottom plane. On the top plane, the potential is prescribed to the given value. The polymer is taken to be isotropic and viscoelastic. The validity of this FE model can be given by the qualitative analysis of temporal evolution of the effective piezoelectric  $d_{33}$  coefficient with respect to various parameters, including the microstructural void parameters, charge density as well as the viscoelastic parameters of polymer. Quantitative comparison was also presented by simulating the experimental results of the effective piezoelectric  $d_{33}$  coefficients of cellular piezoelectret Polypropylene film published in [10], as show in Fig. 3, where the open circles represent experimental results while the solid line is given by this finite element modeling. It can be seen that the simulation agrees fair well with experiments.

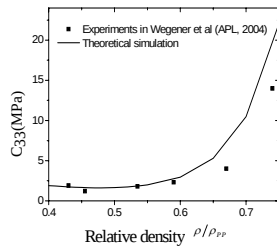


Fig. 1 C33 versus relative density of film

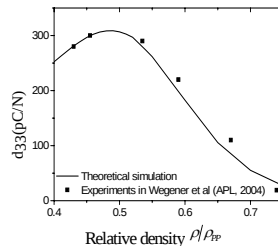


Fig. 2 d33 versus relative density of film

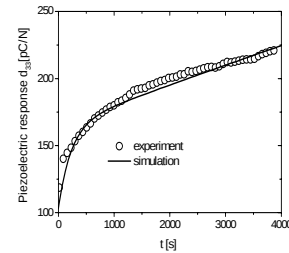


Fig. 3 temporal evolution of d33

## CONCLUSIONS

We have presented a micromechanical model for the prediction of the effective electromechanical properties of cellular piezoelectret film, where the charged voids are deemed as ellipsoidal inclusions. Both qualitative analysis and quantitative comparison with experiment show the validity of this theoretical model. As for the cellular piezoelectret film with more complicated microstructure of voids that are not necessarily of ellipsoidal shape, we developed a finite element model to find the effective piezoelectric coefficient of cellular piezoelectret film. The microvoids are modeled geometrically by the three-dimensional hollow oblate tetrakaidecahedra. Temporal evolution of the effective quasi-piezoelectric  $d_{33}$  coefficient of cellular piezoelectret film is studied. The efficiency of this finite element model can be testified by the analysis of the simulated effective piezoelectric  $d_{33}$  coefficient with respect to various parameters, as well as the comparison with experimental results.

## REFERENCES

- [1]. R. Gerhard-Multhaupt, Less can be More: Holes in Polymers lead to a New Paradigm of Piezoelectric Materials for Electret Transducers, *IEEE Trans. Dielect. Elect. Insul.*, 9, 850-859 (2002)
- [2]. M. Lindner, H. Hoislbauer, R. Schwodiauer, S. Bauer-Gogonea and S. Bauer, Charged Cellular Polymers with "Ferroelectretic" Behavior, *IEEE Trans. Dielect. Elect. Insul.*, 11, 255-263 (2004)
- [3]. J. Hillenbrand and G. M. Sessler, Piezoelectricity in Cellular Electret Films, *IEEE Trans. Dielect. Elect. Insul.*, 7, 537-542 (2000)
- [4]. M. Wegener, W. Wirges, R. Gerhard-Multhaupt, M. Dansachmuller, R. Schwodiauer, M.R. Bauer-Gogonea, S. Bauer, M. Paajanen, H. Minkinen and J. Raukola, Controlled inflation of voids in cellular polymer ferroelectrets: Optimizing electromechanical transducer properties, *Appl. Phys. Lett.*, 84, 392-394 (2004).
- [5]. X. Zhang, J. Hillenbrand, and G.M. Sessler, Improvement of piezoelectric activity of cellular polymers using a double-expansion process, *J. Phys. D Appl. Phys.*, 37 (2004) 2146-2150.
- [6]. J. Hillenbrand, G.M. Sessler, and X. Zhang, Verification of a model for the piezoelectric  $d_{33}$ -coefficient of cellular electret films, *J. Appl. Phys.*, 98, 064105 (2005)
- [7]. G. M. Sessler, and J. Hillenbrand, Electromechanical Response of Cellular Electret Films, *Appl. Phys. Lett.*, 75, 3405-3407 (1999)
- [8]. M. R. Haberman, and Y. H. Berthelot, A differential effective medium model for piezoelectret foams, *J. Appl. Phys.*, 102, 124903 (2007)
- [9]. Y. Wan, L. Xie and Z. Zhong, Micromechanical prediction of the effective electromechanical properties of cellular ferroelectrets, *J. Appl. Phys.*, 108, 054101 (2010)
- [10]. Y. Wan, L. Xie, X. Zhang and Z. Zhong, Time dependence of piezoelectric  $d_{33}$  coefficient of cellular ferroelectret polypropylene film, *Appl. Phys. Lett.*, 98, 122902 (2011)
- [11]. Y. Wan, L. Xie, K. Lou, X. Zhang and Z. Zhong, Experimental and theoretical study on time dependence of the quasi-piezoelectric  $d_{33}$  coefficients of cellular piezoelectret film, 2011, *Journal of the Mechanics and Physics of Solids*, (Submitted)
- [12]. Y. Wan, L. Fan and Z. Zhong, Finite Element Modeling of Temporal Evolution of the Quasi-piezoelectric  $d_{33}$  Coefficient of Cellular Piezoelectret Polypropylene Film, 2011, *Computational Materials Science*, (In press)