Polarization and piezoelectric coefficients of poly(vinylidene fluoride) form-I-films: A model including crystalline orientation

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Expressions for the polarization and the d_{311} and d_{333} piezoelectric coefficients of poly(vinylidene fluoride) form-I-films are derived. The effect of crystallite orientation is included via the orientation distribution function (ODF). In this way the shear piezo effect of the crystal lattice can be taken into account. It has been found also that the odd part of the ODF up to $l = 3$ is significant. With regard to the lamellar structure of the material the crystallites are assumed to be ellipsoidal.

(Keywords: poly(vinylidene fluoride); polarization; piezoelectricity; orientation distribution function; ghost phenomena)

INTRODUCTION

The polarization and piezoelectric coefficients of poly(vinylidene fluoride) (PVDF) form-I single crystals have been calculated by Purvis and Taylor[1,2] and Tashiro *et al.*[3-5] But in the various applications of PVDF, semicrystalline films and not single crystals are used. Therefore a composite effect of crystallites of certain shape dispersed in a non-crystalline (amorphous) matrix must be considered. Infinitely this crystallites acting as rigid dipoles[6] and spherical, ideally oriented crystallites[4,5] have been assumed to exist.

In this paper we attempt to extend the model for calculating the experimental measureable $\tilde{d}^s_{311}$ and $\tilde{d}^s_{333}$ coefficients proposed in ref. 4. Instead of using the assumption of spherical crystallites we will assume that they have an ellipsoidal shape, which allows consideration of the lamellar morphology[6]. The orientation state of the crystalline phase is described using the ODF[7,8]. The first determination of this function from diffraction experiments (pole figure measurements) for biaxially oriented polyethylene (i.e. the general case) was done by Krigbaum *et al.*[9] We have tried to link this function with measurable physical properties. With the help of group theory it is shown that only a few of the ODF components are significant. It should be noticed, however, that these components (except one) cannot be obtained from reduced pole figures due to 'ghost effects'[10]. These effects reflect a loss of information on the ODF in the common pole figures due to the symmetry of the diffraction experiment. The X-rays (or neutrons) cannot distinguish between both sides (top or bottom) of a set of reflecting lattice planes (Friedel's law). The consequences of this fact for the reproduction of ODFs from pole figures are discussed in detail in ref. 7.

POLARIZATION

Proceeding from a two-phase model of PVDF form-I crystallites embedded in an amorphous nonpiezoelectric PVDF matrix, the spontaneous polarization of a suitably oriented film (thickness l, area A) is caused by the permanent electric dipole moment of the crystal lattice in the $\vec{b}$-direction. Throughout this paper we will use a crystallite and a sample co-ordinate system K_B and K_A so that $X_B \| \vec{c}$, $Y_B \| \vec{a}$, $Z_B \| \vec{b}$ and $X_A \|$ stress direction, $Y_A \|$ transverse direction, $Z_A \|$ film normal, respectively. All quantities in K_A are marked with a tilde.

If the crystallites are assumed to have an ellipsoidal shape (lamellar structure[6]), then according to the well known electrodynamic relationship[11] we find that

$$P_3 = P_3^c \varepsilon_a / [\varepsilon_a + n_3(\varepsilon_c^3 - \varepsilon_a)]$$

Here P_3^c is the lattice polarization, P_3 is the lattice polarization modified by the surrounding amorphous material with dielectric constant ε_a. ε_c^3 and n_3 are the third principal axes components of the dielectric and depolarization tensor[11], respectively. If we have N noninteracting equal ellipsoid crystallites, each of volume Ω and polarization $\tilde{\vec{P}}_\nu$ ($\nu = 1, \ldots, N$) the averaged sample polarization is given by

$$\tilde{\vec{P}} = \frac{N\Omega}{Al} \sum_{\nu=1}^{N} \tilde{\vec{P}}_\nu, \qquad |\tilde{\vec{P}}_\nu| = P_3 \tag{1}$$

Now we take into account the crystallite orientation with the help of the ODF $f(g)$[8]. The sum in equation (1) becomes a weighted integral over the whole orientation space G

$$\tilde{\vec{P}} = \frac{N\Omega}{Al} \int_G \tilde{\vec{P}}(g) f(g) \, \mathrm{d}g \tag{2}$$

The factor in front of the integral is simply the crystallinity ϕ. From a mathematical point of view $f(g)$ is a quadratic integrable function on the three-dimensional rotation

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group SO(3), $f(g)\in L^2(\mathrm{SO}(3))$. Thus it can be expressed by a complete and orthogonal system of basis functions. Such a system consists, e.g., of the matrix elements of the irreducible unitary SO(3) representations $D^l_{mn}(g)$ ($l=0, 1,\ldots$; $m,n=-l, -l+1,\ldots,l$) taken in the canonical bases e^l_m (see for example ref. 12). So we have[10]

$$f(g)=\sum_{l=0(1)}^{\infty}\sum_{m,n=-1}^{l} C_l^{mn}D^l_{mn}(g^{-1}) \tag{3}$$

and $D^l_{mn}(g)$ fulfil the orthogonality relations

$$\int_G D^{l'*}_{m'n'}(g)D^l_{mn}(g)\mathrm{d}g=\frac{1}{2\cdot l+1}\delta_{ll'}\delta_{mm'}\delta_{nn'} \tag{4}$$

The rotation group can be parameterized by the three Eulerian angles, α, β, γ usually applied in quantum mechanics[13]. Then $D^1_{00}(\alpha,\beta,\gamma)=\cos\beta$ holds with $D^{l*}_{mn}(g)=D^l_{nm}(g^{-1})$, (3), (4) and $\tilde{P}_3(g)=(\cos\beta)P_3$ we finally get from (2)

$$\tilde{P}_3=\frac{\varepsilon_\mathrm{a}}{\varepsilon_\mathrm{a}+n_3(\varepsilon^3_\mathrm{c}-\varepsilon_\mathrm{a})}P^\mathrm{c}_3\frac{1}{3}C^{00}_1 \tag{5}$$

PIEZOELECTRIC COEFFICIENTS

Next we consider the piezoelectric strain coefficient $\tilde{d}^\mathrm{s}_{311}$ ('s' indicates 'sample')[4]

$$\tilde{d}^\mathrm{s}_{311}=\frac{1}{A}\left(\frac{\partial Q_\mathrm{e}}{\partial\tilde{\sigma}^\mathrm{s}_{11}}\right)_{E=0}=\frac{1}{A}\frac{\partial A\tilde{P}_3}{\partial\tilde{\sigma}^\mathrm{s}_{11}} \tag{6}$$

Q_e is the charge on the covering electrodes and $\tilde{\sigma}^\mathrm{s}_{11}$ is the pure axial stress in X_A direction. The latter equality holds for vanishing electric field in the sample, i.e. for short circuited electrodes.

Also n_{ij} is the tensor whose principal axes components are $\varepsilon_\mathrm{a}/(\varepsilon_\mathrm{a}+n_i(\varepsilon^i_\mathrm{c}-\varepsilon_\mathrm{a}))$ and T_{ij} the matrix transforming K_A into K_B. This means we can consider the rotations as a three-dimensional matrix group, which is itself an orthogonal SO(3) representation T with matrix elements $T_{ij}(g)=T_{ji}(g^{-1})$. Then from equation (2) we get

$$\tilde{P}_3=\phi\int_G T_{3i}(g^{-1})n_{ik}P^\mathrm{c}_k(g)f(g)\mathrm{d}g \tag{7}$$

and P^c_k can further be expressed as

$$P^\mathrm{c}_k(g)=d_{klm}T_{lp}(g)T_{mq}(g)\tilde{\sigma}_{pq}(g)+\delta_{k3}P^\mathrm{c}_3$$

where the crystal piezoelectric strain coefficients d_{klm}[4] have been used. Now also the first and second components of P^c_k are non-zero because the stress deforms the crystal lattice and produces an intrinsic piezo effect. With the assumption of a uniform distribution of stress between the crystalline and amorphous regions (mechanical series (Reuss) model)[14] we find

$$\tilde{\sigma}^\mathrm{s}_{pq}(g)=\tilde{\sigma}_{pq}(g)=\delta_{p1}\delta_{q1}\tilde{\sigma}_{11},\qquad \tilde{\sigma}_{11}=\mathrm{const.} \tag{8}$$

The derivative of $P^\mathrm{c}_k(g)$ yields

$$\frac{\partial P^\mathrm{c}_k(g)}{\partial\tilde{\sigma}^\mathrm{s}_{11}}=d_{klm}T_{l1}(g)T_{m1}(g) \tag{9}$$

and $\tilde{d}^\mathrm{s}_{11}$ in equation (6) is found to be ($\tilde{P}_3$ from equation (5)):

$$\begin{aligned}\tilde{d}^\mathrm{s}_{311}=\tilde{P}_3\Bigg(&-\frac{1}{l}\frac{\partial l}{\partial\tilde{\sigma}^\mathrm{s}_{11}}+\frac{1}{\Omega}\frac{\partial\Omega}{\partial\tilde{\sigma}^\mathrm{s}_{11}}\\ &+\frac{n_3\varepsilon^3_\mathrm{c}}{\varepsilon_\mathrm{a}+n_3(\varepsilon^3_\mathrm{c}-\varepsilon_\mathrm{a})}\left(\frac{1}{\varepsilon_\mathrm{a}}\frac{\partial\varepsilon_\mathrm{a}}{\partial\tilde{\sigma}^\mathrm{s}_{11}}-\frac{1}{\varepsilon^3_\mathrm{c}}\frac{\partial\varepsilon^3_\mathrm{c}}{\partial\tilde{\sigma}^\mathrm{s}_{11}}\right)\Bigg)\\ &+\phi\sum_{i=1}^{3}\frac{\varepsilon_\mathrm{a}}{\varepsilon_\mathrm{a}+n_i(\varepsilon^i_\mathrm{c}-\varepsilon_\mathrm{a})}\int_G T_{3i}(g^{-1})\frac{\partial P^\mathrm{c}_i(g)}{\partial\tilde{\sigma}^\mathrm{s}_{11}}f(g)\mathrm{d}g\end{aligned} \tag{10}$$

In the same way a quite similar equation for $\tilde{d}^\mathrm{s}_{333}$ can be derived. We should remark that the equations (5) and (10) in case of spherical crystallite shape and $f(g)=\partial(g-e)$ (where δ is the delta-distribution and e is the identical transformation) are reduced to the relationships given in ref. 14. Completely new terms appear in the sum of equation (10) for $i=1$ and 2. These contributions involve the shear piezo effect caused by $\tilde{\sigma}_{11}$. According to equation (8) contributions from other σ_{ij} components are neglected. The term with $\tilde{P}_3$ comes from the different properties of the amorphous and crystalline phases and indicates the change of dipole moment per unit volume through composite effects contrary to the sum, which expresses the intrinsic (lattice) effect.

EVALUATION OF THE SIGNIFICANT ODF COMPONENTS

Not all coefficients in the series expansion (equation (3)) are relevant for the piezoelectric 311 and 333 effects analagously to the case of polarization.

We consider the crystal contribution $\tilde{d}^{s(c)}_{311}$in equation (10), written in general co-ordinate system (compare with equation (7)) for recognizing the transformation properties of the integrant

$$\begin{aligned}\tilde{d}^{s(c)}_{311}&=\phi\int_G T_{3i}(g^{-1})n_{i\mathrm{h}}\frac{\partial P^\mathrm{c}_\mathrm{h}(g)}{\partial\tilde{\sigma}^\mathrm{s}_{11}}f(g)\mathrm{d}g\\ &=\phi\int_G T_{3i}(g^{-1})n_{ih}d_{hjk}T_{j1}(g)T_{k1}(g)f(g)\mathrm{d}g\\ &=\phi\sum_{l,m,n}\int_G T_{3i}(g^{-1})T_{j1}(g)T_{k1}(g)n_{ih}d_{hjk}C^{mn}_l D^l_{mn}(g)\mathrm{d}g\end{aligned}$$

where equations (9) and (3) have been used. Introducing the third-rank tensor $A_{ijk}=n_{ih}d_{hjk}$ the integrant becomes

$$T_{3i}(g^{-1})T_{1j}(g^{-1})T_{1k}(g^{-1})A_{ijk}C^{mn}_l D^l_{mn}(g^{-1})$$

In order to exploit equation (4) we have to find the irreducible parts of the tensor product representation $T\otimes T\otimes T$acting on the third-rank tensors ltA. If we deal with a product of unitary irreducible SO(3) representations D^l this problem would be solved by the well known (real) Clebsch–Gordan coefficients $(l_1l_2m_1m_2|lm)$[12]

$$e^l_m=\sum_{m_1+m_2=m}(l_1l_2m_1m_2|lm)e^{l_1}_{m_1}\otimes e^{l_2}_{m_2}$$

From $\dim T = \dim D^1$ ($=3$), $\dim D^l \neq 3$ for $l \neq 1$ and the fact that both representations are irreducible, they must be equivalent:

$$T = V^{-1} D^1 V$$

In the bases e^1_m and e_i (orthonormal cartesian basis in R^3) V becomes

$$V_{mi} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \qquad (11)$$

The tensor product definition yields

$$\begin{aligned}(T \otimes T \otimes T)A &= ((V^{-1}D^1 V) \otimes (V^{-1}D^1 V) \otimes (V^{-1}D^1 V))A \\ &= ((V^{-1} \otimes V^{-1} \otimes V^{-1})(D^1 \otimes D^1 \otimes D^1) \\ &\quad \times (V \otimes V \otimes V))A\end{aligned}$$

with the common Clebsch–Gordan problem

$$D^1 \otimes D^1 \otimes D^1 = D^0 \oplus 3\mathbf{D}^1 \oplus 2D^2 \oplus D^3$$

With the unitarity condition

$$\sum_{m_1} (l_1 l_2 m_1 m_2 | lm)(l_1 l_2 m_1 m_2 | l'm') = \delta_{ll'} \delta_{mm'}$$

the following explicit formula can be derived

$$(T \otimes T \otimes T)A = \sum_{l,m,n} \{rst;lmn;ijk\} A_{ijk} D^l_{nm} e_r \otimes e_s \otimes e_t,$$

$$\{rst;lmn;ijk\} := \sum_{l',_i,n_i} ({}_{m_1 i} V_{m_2 j} V_{m_3 k} V^{-1}_{rn_1} V^{-1}_{sn_2} V^{-1}_{tn_3}) \qquad (12)$$

$$(11\, m_2 m_3 | l' \mathrm{m}_{23})(1\, l' m_1 m_{23} | lm)(11\, n_2 n_3 | l' n_{23})(1\, l' n_1 n_{23} | ln))$$

Here the sum must be taken according to the relations

$l' = |l-1|, |l-1|+1, \ldots, \min(2,l+1)$; $m_1 + m_{23} = m$; $m_2 + m_3 = m_{23}$; $m_i = -1, 0, 1$; analogically for n_i. Some symmetries of the Clebsch–Gordan coefficients[12] and equation (11) yield

$$\begin{aligned}\{rst; l-mn; ijk\} &= (-1)^{1+l+i_1+j_1+k_1} \{rst; lmn; ijk\} \\ \{rst; lm-n; ijk\} &= (-1)^{1+l+r_1+s_1+r_1} \{rst; lmn; ijk\} \qquad (13)\end{aligned}$$

$$i_1 = \begin{cases} 1 \text{ for } i = 1 \\ 0 \text{ for } i = 2,3 \text{ etc.} \end{cases}$$

CRYSTAL AND SAMPLE SYMMETRIES

Due to the present choice of axes, the PVDF form-I space group reads *Amm*2 and its point group *mm*2. Therefore, only those tensor components are not zero that belong to the subspace transforming according to the trivial representation of the point group. For *mm*2 and with $A_{ijk} = A_{ikj}$ these components are A_{113}, A_{223}, A_{311}, A_{322}, A_{333} [15].

Tables 1 and *2* show the results from the evaluation of equation (12). All other coefficients except those gained from equation (13) are zero. The point group also affects the series expansion (equation (3)). In the notation of Matthies[7,10] we deal with a type III crystal class. The crystal symmetry of the true ODF is $G_B = C_2$:

$$T^L_{h_i^{-1}} f(g) = f(h_i g) = f(g);\ hi \in C_2;\ i = 1,2 \qquad (14)$$

The rotational part G_A of the sample symmetry of a piezoelectric (poled) film is also C_2 with the axis normal to the film:

$$T^R_{h_i} f(g) = f(gh_i) = f(g);\ h_i \in C_2;\ i = 1,2 \qquad (15)$$

Here we introduce the left and right regular representations T^L and T^R of C_2[16], respectively. With the help of the linear independence of the $D^l_{mk}(g)$ from equations (14) and (3) we get for any l and n

$$\begin{aligned}\sum_k D^l_{kn}(h_i^{-1}) \sum_m C^{mn}_l D^l_{mk}(g^{-1}) &= \sum_m C^{mn}_l D^l_{mn}(g^{-1}) \\ &= \sum_k \delta_{kn} \sum_m C^{mn}_l D^l_{mn}(g^{-1})\end{aligned}$$

That means we look for such linear combinations of basis elements $D^l_{mk}(g^{-1})$ on which $T^L_{h_i}$ acts as the trivial representation δ_{kn}. These can easily be obtained with the projection operator formalism[12] and $D^l_{mn}(e) = \delta_{mn}$, $D^l_{mn}(C_2) = (-1)^m \delta_{mn}$. One finds a selection rule for the index m: $m = 0, \pm 2, \pm 4, \ldots$ The complete decompositions of the regular representations of all point groups up to $l = 8$ are tabulated in ref. 17. In the present case the relations (14) and (15) obviously do not give a further elimination of ODF components.

PIEZOELECTRIC COEFFICIENTS (SUM FORM)

Now the orthogonality relations (4) can be used to simplify the crystal contribution $\tilde{d}^{s(c)}_{311}$ in equation (10). With equations (10), (9) and (3) we have (principal axes)

$$\begin{aligned}\tilde{d}^{s(c)}_{311} = \phi \sum_{i=1}^{3} \frac{\varepsilon_a}{\varepsilon_a + n_i(\varepsilon^i_c - \varepsilon_a)} \sum_{l,m,n} \int_G T_{3i}(g^{-1}) T_{ij}(g^{-1}) T_{ik}(g^{-1}) d_{ijk} \\ \times C^{mn}_l D^l_{mn}(g^{-1}) \mathrm{d}g\end{aligned}$$

and with equation (12)

$$\begin{aligned}\tilde{d}^{s(c)}_{311} = \phi \sum_{i=1}^{3} \frac{\varepsilon_a}{\varepsilon_a + n_i(\varepsilon^i_c - \varepsilon_a)} \sum_{\substack{l,m,n \\ l',m',n'}} \{311; l'm'n'; ijk\} d_{ijk} C^{mn}_l \\ \times \int_G D^{l'}_{n'm'}(g^{-1}) D^l_{mn}(g) \mathrm{d}g\end{aligned}$$

The relation (4) and $D^l_{mn}(g) = (-1)^{m-n} D^{l*}_{-m-n}(g)$ yield

$$\begin{aligned}\tilde{d}^{s(c)}_{311} &= \phi \sum_{i=1}^{3} \frac{\varepsilon_a}{\varepsilon_a + n_i(\varepsilon^i_c - \varepsilon_a)} \\ &\quad \times \sum_{l,m,n} \{311; l-n-m; ijk\} d_{ijk} \frac{(-1)^{m-n} C^{mn}_l}{2l+1} \qquad (16)\end{aligned}$$

analogically for $\tilde{d}^{s(c)}_{333}$. The sum (equation (16)) is finite and must be taken according to *Table 1* and equation (13). The C^{mn}_l ($l \leqslant 3$) contain the features of the texture, important for the piezo effect. But at the moment there is no common simple experiment to determine the coefficients

Table 1 Nonvanishing {311; *lmn*; *ijk*}

i j k	1 1 3	2 2 3	3 1 1	3 2 2	3 3 3
l m n					
1 0 0	−1/10	−1/10	2/5	2/5	1/5
2 2 2	−1/12	1/12	1/6	−1/6	0
3 0 0	1/10	1/10	1/10	1/10	−1/5
3 0 2	$-\sqrt{30}/60$	$-\sqrt{30}/60$	$-\sqrt{30}/60$	$-\sqrt{30}/60$	$+\sqrt{30}/30$
3 2 0	$-\sqrt{30}/60$	$\sqrt{30}/60$	$-\sqrt{30}/60$	$\sqrt{30}/60$	0
3 2 2	1/12	−1/12	1/12	−1/12	0

Table 2 Nonvanishing {333; *lmn*; *ijk*}

i j k	1 1 3	2 2 3	3 1 1	3 2 2	3 3 3
l m n					
1 0 0	1/5	1/5	1/5	1/5	3/5
3 0 0	−1/5	−1/5	−1/5	−1/5	2/5
3 2 0	$\sqrt{30}/30$	$-\sqrt{30}/30$	$+\sqrt{30}/30$	$-\sqrt{30}/30$	0

with odd values of l. This represents a still open problem of the whole quantitative texture analysis, which also occurs in metal physics. The C_l^{mn} with even l can be obtained by the classical Bunge–Roe method[8,9].

CONCLUSIONS

Polarization and piezoelectric coefficients are examples physical properties depending on the odd part of the ODF[7,10]. Therefore we are confronted with ghost effects, namely with special, uncorrectable ghosts. That means that with common pole figure experiments only an ODF of higher crystal symmetry (D_2) can be reproduced. Taking into account anomalous scattering, unreduced pole figures can be obtained in principle. But as there are only light atoms in the unit cell the effect seems not large enough to be experimentally utilized. For instance the Bijvoet-ratio[18] of the (110) reflection and CrKα radiation is only about 3%.

The calculations of 'Evaluation of the significant ODF components' are applicable to tensors of any rank and, therefore, can also be applied to dielectrical (second-rank) and mechanical (fourth-rank) properties. It must be clarified in each case if the even part of the ODF is sufficient to describe the property considered.

With the assumption of ellipsoidal crystallites in 'Polarization' further information about lamellae dimensions can be utilized in the model by an appropriate principal axes ratio.

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