

Preisach modeling of the electric-field-induced strain of ferroelectric material

プライザツハモデルによる強誘電体の電界誘起歪のモデル化

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1. Introduction

Preisach model is a powerful tool to study a hysteresis behavior. Many researches have been performed to apply this model to the ferromagnetic system [1] and also ferroelectric system [2]. In ferromagnetism, it successfully describes the hysteresis behavior. The polarization hysteresis loop of the ferroelectric material is also described by Preisach model. However, there are few reports that study the Preisach modeling of the field-induced strain hysteresis of the ferroelectric materials [3]. This is because the strain hysteresis is mainly affected by the non-180° domain switching process, which had not been treated by the classical Preisach model. In this research, we propose an improved Preisach model that includes non-180° domain switching and the modeling of the strain hysteresis is demonstrated.

2. Classical and Improved Preisach model

The classical Preisach model was composed of the hysteresis loop as the parallel connection of independent relay hysterons. A classical relay hysteron is shown in **Fig.1 (a)**. The rectangular hysteron is defined with two parameters, switching down fields Y and switching up fields X . The value of the hysteresis operator is $+p$ or $-p$ which indicates the magnetic or electric polarization direction. When the field E is $Y \leq E \leq X$, the value of the hysteresis operator depends on its past state. It results in the hysteresis behavior. The hysterons which have different X and Y are given weights. The weight function which is called Preisach distribution function features the whole hysteresis loop.

When the ferroelectric material is composed of tetragonal phase, the polarization directions are not only up and down, but also horizontal directions that along with the plane perpendicular to the z -axis. In z direction, the polarization has three states as $+p$, 0 , and $-p$. Concerning the strain, there are two states according to its polarization state. Assuming the strain at 0 polarization state as 1 , the strain at $+p$ or $-p$ is c/a , where c and a are lattice constants of the

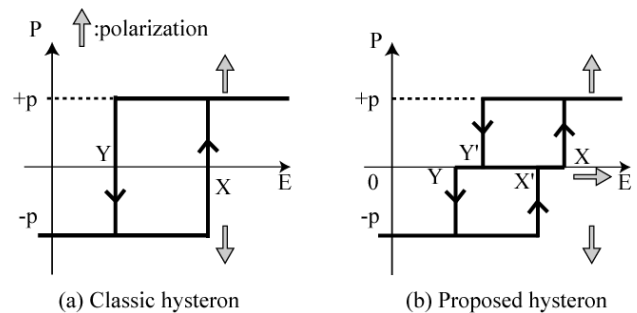


Fig. 1 Hysteresis relay operators (a) classic hysteron, (b) proposed hysteron.

tetragonal cell. This strain is the non-180° domain switching strain.

Then, we propose a new hysteresis operator that has three states as $+p$, 0 , and $-p$ shown in **Fig.1 (b)**. This hysteron is defined by four parameters, Y as switching down field to $-p$, X as switching up field to $+p$, Y' as switching down field to 0 , X' as switching up field to 0 . These parameters follow $X \geq X' \geq Y' \geq Y$. A unique hysteron is defined with X , X' , Y and Y' . Then a XY plane and huge number of $X'Y'$ plane is considered as shown in **Fig.2**. At a certain point (x, y) in XY plane, certain number of hysterons exist which have various X' and Y' parameters respectively. A $X'Y'$ plane is defined in $X' \leq x, y \leq Y'$. In this $X'Y'$ plane, a unique hysteron with x, y, x', y' is determined. In this proposed model, not only a weight function in XY plane, but also that in $X'Y'$ plane features the whole hysteresis behavior. The whole polarization or strain states are obtained by the integration of these weight functions.

3. Calculation method

Figure 2 shows how we calculate the polarization change under certain electric field. **Fig.2 (a)** denotes polarization change when electric field increases to be E_{inc} . The initial polarization states are assumed to be all $-p$. In the XY plane, if $X < E_{inc}$, all corresponding hysterons in $X'Y'$ plane becomes $+p$. Where $X > E_{inc}$, they don't become $+p$ but some of them becomes 0 from $-p$. Considering about a $X'Y'$ plane with a point (x, y) with $x > E_{inc}$, in the plane, points with $x' \leq E_{inc}$ become 0 . This

switch corresponds to the non-180° domain switching. It should be noted the point where its value is +p does not become 0 though $x' \leq E_{inc} < x$, because the up polarization direction won't change when electric field is increasing.

Subsequently, **Fig.2 (b)** denotes the polarization change, when electric field decreases to E_{dec} . The polarization state will change in the same manner. In the $X'Y'$ plane, if $Y > E_{dec}$, all corresponding hysterons in $X'Y'$ plane becomes $-p$. In the XY plane, where $Y \leq E_{dec}$, they don't become $-p$, but become 0 from $+p$. Considering about a $X'Y'$ plane with a point (x, y) with $y < E_{dec}$, in the plane, points with $y' \geq E_{dec}$ becomes 0 except for the point of $-p$. In this manner, the polarization change under electric field is calculated.

The whole polarization P is calculated as

$$P = \iint_{S_{+p}} \iint_{S_{+p}} K(x, y) K'_{x,y}(x', y') dx' dy' dx dy - \iint_{S_{-p}} \iint_{S_{-p}} K(x, y) K'_{x,y}(x', y') dx' dy' dx dy,$$

where $K(x, y)$ and $K'_{x,y}(x', y')$ are Preisach distribution functions of XY and of $X'Y'$ plane. The subscripts of $K'_{x,y}(x', y')$ indicates that it is a function of x and y . The distribution functions $K'_{x,y}(x', y')$ exit huge numbers. Thus, to treat the distribution function easily, a distribution function $K'(X', Y')$ is defined. The value of the distribution function $K'(X', Y')$ at (x', y') satisfies

$$K'(x', y') = \iint K'_{x,y}(x', y') dx dy.$$

Then, the whole hysteresis behavior is featured by $K(x,y)$ and $K'(x',y')$. The domain switching strain S_{DS} is calculated as

$$S_{DS} = \frac{\iint_{S_{+p}+S_{-p}} \iint_{S_{+p}+S_{-p}} K(x, y) K'_{x,y}(x', y') dx' dy' dx dy}{\iint \iint K(x, y) K'_{x,y}(x', y') dx' dy' dx dy} \times \frac{c}{a}.$$

4. Results

We assumed a pseudo Voigt function and a Cauchy function as the distribution functions for example. The calculated polarization hysteresis loop and strain hysteresis loop are obtained as shown in **Fig.3**. The hysteresis loop and butterfly shaped strain hysteresis are successfully simulated.

5. Conclusion

In this work, an improved Preisach model was proposed, which includes the non-180° domain switching effect. We demonstrated the Preisach calculation with the new hysteresis operator.

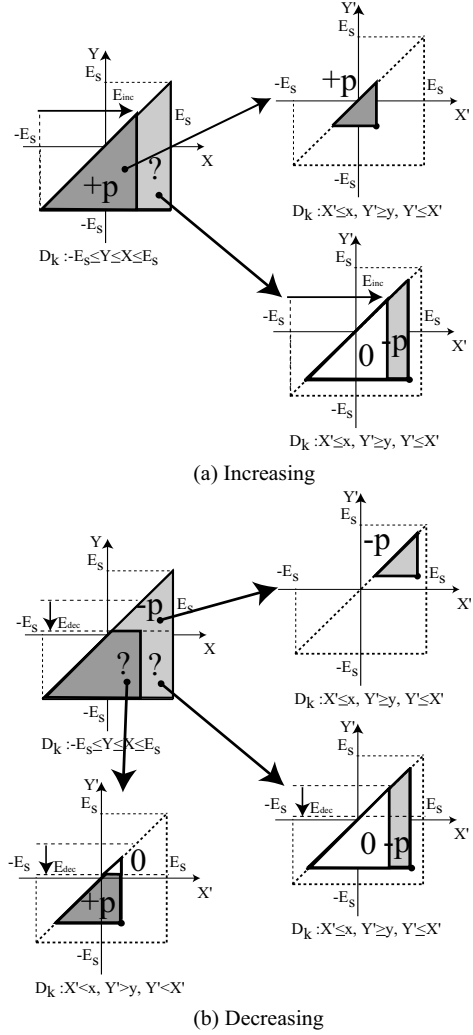


Fig. 2 Calculated methods (a) when electric field is increasing, (b) when electric field is decreasing.

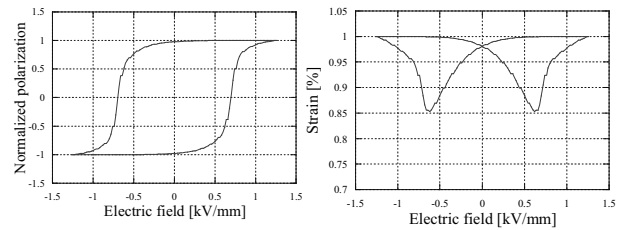


Fig. 3 Calculated (a) polarization hysteresis and (b) strain hysteresis.

Acknowledgment

This work was supported by Grant-in-Aid for JSPS Fellows, No. 216357.

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