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Estimation of toughening produced by ferroelectric/ferroelastic domain switching

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Abstract

An estimate is made of the upper limit of the toughening that might be expected by the crack tip stress induced reorientation of domains in ferroelectric ceramics. The calculation is based on obtaining the shielding stress intensity factor produced by the shear transformation of a zone surrounding the crack tip and extending over the crack surfaces. The estimate suggests that the toughening that might be expected is less than 10% even in the most ideal conditions. This case is contrasted with the much greater toughening which is expected from the crack tip stress induced phase transformations which are largely driven by the chemical, or bulk, free energy change of the transformation. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Ferroelectric; Fracture

1. Introduction

The length of the cracks formed at the corners of a Vickers indentation on the surface of lead zirconate titanate (PZT) is greatly influenced by both the poling condition of the material and the poling direction with respect to the orientation of the cracks.[1–5] It has been proposed that this fracture toughness anisotropy arises from the crack tip stress induced switching, or reorientation, of the non-180° ferroelectric domains which can occur at the tip of cracks growing in a plane parallel to the poling direction but not at the tip of cracks growing in a plane normal to the poling direction.[2,3] The occurence of R-curve behaviour in $BaTiO_3$[6] and PZT[7] has also been attributed to ferroelastic switching.

In this paper we attempt to estimate the toughening that might be expected from the stress induced domain switching at the tip of cracks in a ferroelectric/ferroelastic material.

2. Calculation of the shielding stress intensity factor

The rotation or switching of the domains is achieved by a deformation twinning mechanism, which is effectively a local plastic deformation. The toughening that this produces can be estimated by calculating the associated crack shielding stress intensity factor.

We consider an idealised model in which the material is considered to be perfectly poled parallel to the crack growth direction, so that all of material can potentially switch and contribute to the toughening mechanism. We make several assumptions, all of which have the effect of overestimating the potential toughening. The result that we obtain therefore represents an upper limit for the possible toughening that might be expected. The twinning deformation is assumed to be activated by the resolved crack tip induced 45° shear stresses[8] (Fig. 1):

$$\tau_{45} = \left(\sigma_y - \sigma_x\right)/2 = \left(K_1/2\sqrt{2\pi r}\right)\sin\theta\sin(3\theta/2) \quad (1)$$

The shape of the transformation zone is shown in Fig. 2. The width of the zone, w, corresponds to the maximum distance over which some critical shear stress, τ_c, to produce the transformation is achieved:

$$w = r_c\sin\theta_c = (0.1/\pi)(K_1/\tau_c)^2 \quad (2)$$

where $\theta_c = 72°$ is the angle that maximises the zone width. We assume that there is no reverse switching in the crack wake, although there is good evidence to suggest that this occurs.[9]

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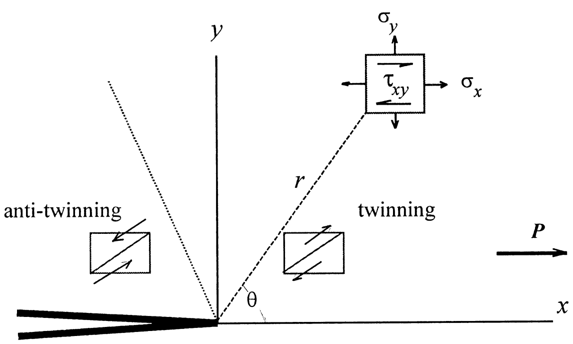

Fig. 1. Crack tip stresses.

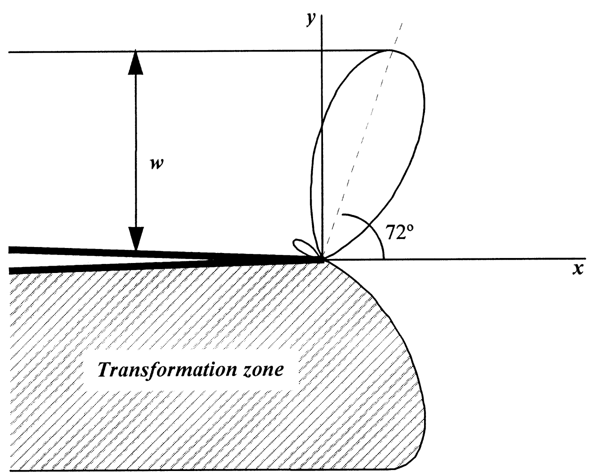

Fig. 2. Shape of transformation zone for ferroelectric/ferroelastic switching.

The stress intensity produced by the transformation can be calculated by the Eshelby procedure and the weight function method.[10,11] This is obtained from the solution of the integral:

$$\Delta K = \int_s \boldsymbol{t}_i \cdot \boldsymbol{m}(x, y)\mathrm{d}S \tag{3}$$

where $\boldsymbol{m}(x,y)$ is the two dimensional relevant weight function and the integral is over the surface of the transformed region. The tractions, $\boldsymbol{t}$, are the surface tractions that would be needed to produce an elastic unconstrained shear, and are equal and of opposite sign to those which would restore the deformed region to its original shape (Fig. 3).

The components of the tractions in the y-direction, t_y, that give rise to the to ΔK_I are the same as those that would be produced by a hydrostatic stress of magnitude $p=\tau$. This coincidence makes it possible to use the solutions available for the crack tip shielding, ΔK_I, produced by a zone experiencing a symmetrical volume expansion.[11,12]

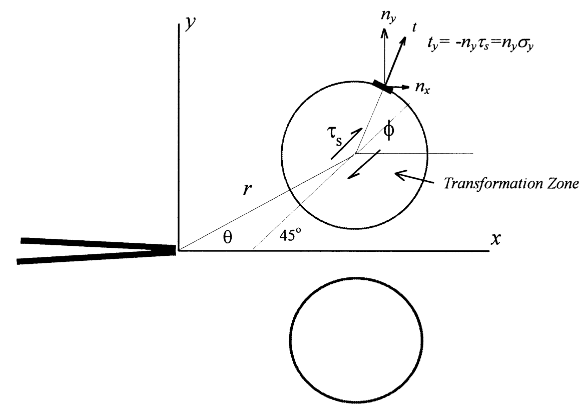

Fig. 3. Tractions produced by a shear transformation.

3. Phase transformation

The problem of the toughening produced by a transformed zone, under a hydrostatic pressure, p, resulting from a volume expansion, and extending over the crack surfaces, was solved by McMeeking and Evans[11] for the t–m transformation of zirconia.

The maximum asymptotic value for the shielding stress intensity factor obtained from their calculation is, when the positive contribution of the frontal transformation zone is included in the calculation:

$$\Delta K_\mathrm{I}/E\varepsilon_\mathrm{p}V_\mathrm{f}\sqrt{w} = -0.22/(1-\nu) \tag{4a}$$

and is, when the contribution of the frontal zone is neglected:

$$\Delta K_\mathrm{I}/E\varepsilon_\mathrm{p}V_\mathrm{f}\sqrt{w} = -0.37/(1-\nu) \tag{4b}$$

where E and ν are the Young's modulus and Poisson's ratio of the material respectively, ε_p is the unconstrained volumetric transformation strain, and V_f is the volume fraction of material that has transformed. These solutions can be applied to the shear transformation problem if the appropriate conversions are made. The shape of the frontal lobes zones for the volume and shear transformations are very different (Figs. 2 and 4). Therefore, Eq. (4b) is applicable for the shear transformation problem.

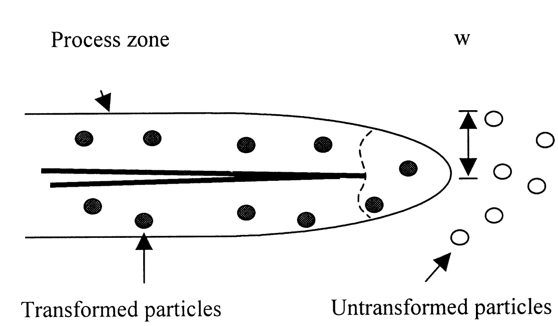

Fig. 4. Shape of transformation zone for volumetric phase transformation.

The relation between the constrained hydrostatic stress, p, and the stress free volumetric strain, ε_p, for the volume expansion is:

$$p = E\varepsilon_p/3(1-2\upsilon) \quad (5)$$

So, if ν is taken as 1/3:

$$p = E\varepsilon_p \quad (6)$$

4. Ferroelastic switching

For a homogeneously sheared region, the relation between the constrained shear stress and the stress free shear strain, γ, is given by:[13,14]

$$\tau_T = 2\beta\mu\gamma \quad (7)$$

where $\beta = (7-5\nu)/15(1-\nu)$ is the constraint factor and μ is the shear modulus. The transformation stress opposes the crack tip stress activating the transformation. If ν is taken as 1/3:

$$\tau_T = 0.4E\gamma \quad (8)$$

Therefore, if Eq. (4b) is to be used for the shear problem, with the stress free transformation shear strain, γ, in place of the volumetric strain, ε_p, the right hand side has to be multiplied by 0.4 to give:

$$\Delta K_I/E\gamma V_f\sqrt{w} = -0.148/(1-\nu) \quad (9)$$

where the product γV_f in this equation is the unconstrained effective transformation strain, γ_e, resulting from the reorientation of a certain volume fraction of domains.

Since the effective transformation strain is a function of the crack tip stress activating it, the transformation zone around the crack tip will consist of a discrete inner region where the crack tip stress has exceeded some critical stress and has experienced the maximum uniform unconstrained transformation strain, γ. This will be surrounded by an outer region which is plastically relaxed by a non uniform transformation strain which decreases to zero. To simplify this complex situation, we will assume that the transformation zone is homogeneously transformed with the unconstrained transformation strain, γ, and that the width of the zone is determined by the critical shear stress, γ_c, needed to activate the transformation.

The crack tip shear stress, τ, required to produce a given transformation strain is not equal to the coercive shear stresses, τ', needed to produce the same irreversible strain in compression. The transformation of the material around the crack tip is constrained and opposed by the uniform transformation stress, τ_T, given by Eq. (8), whereas in compression tests the deformation is mechanically unconstrained. Therefore, unless the crack tip stress τ exceeds τ_T there can be no transformation. The crack tip stress needed for transformation is then:

$$\tau = \tau_T + \tau' \quad (10)$$

The difference, $\tau - \tau_T$ can be regarded as the effective stress activating the transformation.

Substituting for w from Eq. (2) into (9):

$$\Delta K_I/K_I = -0.038E(\gamma V_f/\tau) \quad (11)$$

which can be taken with its positive value if $\Delta K_I/K_I$ is defined as the toughening or relative toughness increase produced by the domain rotation.

Assuming that all of the material in the transformation zone switches, so that $\gamma_e = \gamma$, and $\tau' = 0$, an upper bound estimate for the toughening can be obtained. Substituting for τ_T from Eq. (8) into (11) gives:

$$\Delta K_I/K_I = 0.1 \quad (12)$$

5. Discussion and conclusions

We have presented an overestimate of the maximum contribution that crack tip stress-induced domain rotation could make to the fracture toughness of a ferroelectric/ferroelastic material. This contribution is less than 10% even in the most favourable conditions. This result contrasts with the much more significant toughening that can be produced in zirconia materials where the transformation of the metastable tetragonal phase to the monoclinic phase has a chemical driving potential that helps to overcome the transformation stress, which opposes the domain reorientation. For the ferroelastic toughening, where the transformation is exclusively driven by the crack tip stress field, the toughening is limited by the fact that the transformation stress increases proportionally with the transformation strain. The width of the transformation zone, however, varies with the effective strain, γV_f.

Acknowledgements

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References

1. Yamamoto, T., Igarishi, H. and Okazaki, K., Mechanical properties of (Pb,Ca)TiO_3 family ceramics with zero planar coupling factor. *Ceram. Int.*, 1979, **11**, 75.

2. Pisarenko, G. G., Chushko, V. M. and Kovalev, S. P., Anisotropy of fracture toughness of piezoelectric ceramics. *J. Am. Ceram. Soc.*, 1985, **68**, 259–265.
3. Mehta, K. and Virkar, A., Fracture mechanisms in ferroelectric-ferroelastic lead zirconate titanate (Zr:Ti = 0.54:0.46) ceramics. *J. Am. Ceram. Soc.*, 1990, **73**, 567–574.
4. Zhiwu, Z. and Raj, R., Influence of grain size on ferroelastic toughening and piezoelectric behaviour of lead zirconate titanate. *J. Am. Ceram. Soc.*, 1995, **78**, 3363–3368.
5. Guiu, F., Hahn, B. S., Lee, H. L. and Reece, M. J., Growth of indentation cracks in poled and unpoled PZT. *J. Eur. Ceram. Soc.*, 1997, **17**, 505–512.
6. Meschke, F., Raddatz, O., Kolleck, A. and Schneider, G. A., R-Curve behaviour and crack closure stresses in barium titanate and (Mg,Y)–PSZ ceramics. *J. Am. Ceram. Soc.*, 2000, **83**, 353–361.
7. Lucato, S., Lupascu, D. C. and Rodel, R., Effect of poling direction on R-curve behaviour in lead zirconate titanate. *J. Am. Ceram. Soc.*, 2000, **83**, 424–426.
8. Ewalds, H. L. and Wanhill, R. J. H., *Fracture Mechanics*. Edward Arnold, London, 1991.
9. Cao, H. and Evans, A. G., Nonlinear deformation of ferroelectric ceramics. *J. Am. Ceram. Soc.*, 1993, **76**, 890–896.
10. Bueckner, H. F., A novel principle for the computation of stress intensity factors. *Z. Angew. Meth. Mech.*, 1972, **50**, 529–533.
11. McMeeking, R. M. and Evans, A. G., Mechanics of transformation-toughening in brittle materials. *J. Am. Ceram. Soc.*, 1982, **65**, 242–246.
12. Li, C. M. and Sanday, S. C., Dispersion toughening. *Acta Metall.*, 1986, **34**, 537–543.
13. Eshelby, J. D., The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proc. Roy. Soc. A*, 1957, **241**, 376–396.
14. Brown, L. M. and Stobbs, The fatigue hardening and softening of copper containing silica particles. *W. M., Phil. Mag.*, 1971, **23**, 1169–1184.