Concerning the correlation between dielectric breakdown field strength and lattice constant in alkali halides

Vijh [1] has recently illustrated the existence of a correlation between dielectric breakdown field and lattice constant in alkali halides, i.e. a smaller lattice constant leads to a larger breakdown field. This correlation was qualitatively rationalized on the basis that a larger lattice constant implies poorer solid state cohesion and hence a lower value of the dielectric breakdown field. The purpose of the present note is to show that the observed correlation is quite reasonable when one considers the dependence of band-gap width on lattice constant and the physical mechanisms of dielectric breakdown.

It is well known that breakdown begins with the appearance of electrons in the conduction band. At high fields these electrons achieve high velocities and by collisions transfer part of their energy to valence electrons, which may then be excited to the conduction band. Above a certain critical field, known as the dielectric breakdown field F, an avalanche of electrons into the conduction band is produced. Thus, one expects that the important parameter in determining the dielectric breakdown field would be the energy gap E_g. For smaller values of the energy gap one has correspondingly smaller breakdown fields. Indeed, Vijh [1] mentions that he has previously [2] found such a correlation between dielectric breakdown field and energy gap for the alkali halides; however, an examination of this paper failed to find a mention of such a correlation.

TABLE I

Compound	F_{exp} (MV cm^{-1})*	E_g (eV)†	$-U_c$ (kcal mol^{-1})‡
LiF	3.1	12	242.3
NaF	2.4	⩾10.5 (~11^d)	214.4
KF	1.9	10.9	189.5
NaCl	1.5	8.6	182.6
NaBr	0.81	7.7	173.6
KCl	1.0	8.5	165.8
RbCl	0.83	8.2	159.3
KBr	0.70	7.8	158.5
RbBr	0.63	7.7	152.6
KI	0.57	⩾ 6.2 (~7.4§)	149.9
RbI	0.49	⩾ 6.1 (~7§)	144.9

* [1]
† [8]
‡ [9]
§Determined from Fig. 1. The approximate relation Equation 1 gives the values 11.2, 6.9, and 6.6 for NaF, KI, and RbI, respectively.

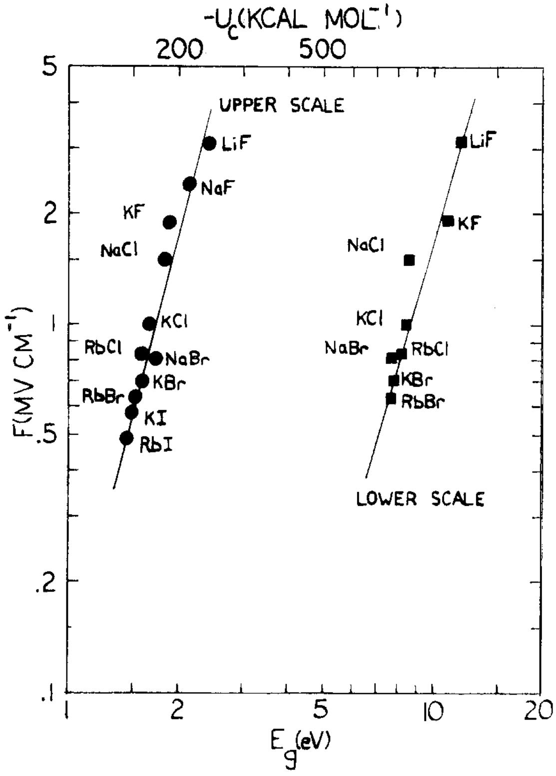

Figure 1 Log–log plot of the dielectric breakdown field strength versus energy gap width (■) and cohesive energy (●).

Fig. 1 shows a convenient log–log plot of F versus E_g, in which it is readily observed that a direct correlation

$$F \approx 1.7 \times 10^{-3} E_g^3 \qquad (1)$$

between dielectric breakdown field and energy gap exists and is consistent with the ideas set forth above. The slope of the line, which was drawn as a visual best fit of the data, is approximately 3. The values of several pertinent parameters for the alkali halides are listed in Table I. It may well be that Equation 1 or Fig. 1 could be used to predict energy gaps from experimental breakdown fields or vice versa, indicating its overall usefulness.

In light of the correlation in Fig.1 and Equation 1, one can now show that the F-a (lattice constant) correlation, illustrated by Vijh, is reasonable. It has been shown by Harrison and Ciraci [3, 4] that

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within the bond-orbital model the nearest neighbour bonding matrix element has a d^{-2} dependence on bond length. This relation was also found to hold for other nearest-neighbour matrix elements [5], and Pantelides [6] has extended these ideas to show that

$$E_g = N_g (\hbar^2 d^{-2}/m) \quad (2)$$

where N_g is a dimensionless constant called the band-gap index. For the alkali halides it was shown that $N_g = 9.1$. N_g is a function only of the chemical valence of the constituent atoms and obeys the empirical relation

$$N_g = N_{go} - 3.8Z \quad (3)$$

where N_{go} is the band gap index of the rare gas solids, 12.9, and Z the valence [6]. Pantelides [6] has shown that Equation 2 is obeyed for a wide range of materials–rare gas solids, alkali halides, chalcogenides, and pnictides. Thus, on the basis of Equations 1 and 2, it is readily seen that a relation

$$F = Ba^{-6} \quad (4)$$

exists where $B = 1.7 \times 10^{-3} (N'_g \hbar^2/m)^3$ and N'_g is a new band-gap index which accounts for the relation between bond length and lattice constant for these solids. It can be seen that Equation 4 is qualitatively consistent with Vijh's correlation.

It was previously mentioned that Vijh rationalized the correlation between F and a by considerations of solid state cohesion. Figure 1 also shows a plot of F versus cohesive energy, indicating that such an approach is reasonable. However, we feel that our approach is certainly physically meaningful when one considers the physical phenomena occurring at dielectric breakdown, i.e. the width of the energy gap is the pertinent parameter. For a complete review of dielectric breakdown in solids, see the article by O'Dwyer [7].

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Fracture mode transitions in polymethylmethacrylate

A recent paper [1] described measurements on the fracture behaviour of polymethylmethacrylate (PMMA) in the crack-speed range 10^{-3} to 10^{0} m sec^{-1}, and discussed the transition from slow stable crack propagation to fast unstable crack propagation that occurs in PMMA, at room temperature, at approximately 2×10^{-2} m sec^{-1}. Various explanations of this transition were referred to, including a change in the mode of formation of crazes ahead of the crack tip from one plane at low velocities, to a multiplane mode at higher velocities [2]. This fracture mode change was described in [2] to explain the transition between the macroscopically smooth surface and the striated macroscopically rough surface that occurs in PMMA in the fracture velocity range 400 to 500 m sec^{-1}. Consequently, the comment in [1] that the multiplane crazing explanation was inconsistent with observed features on the lower speed stable/unstable fracture transition is hardly surprising.

A further effect was suggested in [2], that the stable/unstable fracture transition at low speeds is a change from the process of formation of a single, coherent well-defined craze ahead of the crack, and its subsequent splitting, at low crack speeds; to the formation of numbers of crazes ahead of the crack tip and their subsequent coalescence at higher speeds. Below crack speeds of approximately 400 m sec^{-1}, these crazes are formed substantially on

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