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Intrinsic Breakdown Strength: Theoretical Derivation and First-Principles Calculations

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Abstract: Intrinsic breakdown strength (F_{bd}), as the theoretical upper limit of electric field strength that a material can sustain, plays important roles in determining dielectric and safety performance. The well accepted concept is that a larger band gap (E_{g}) often leads to a larger intrinsic breakdown strength. In this work, we analytically derive a simplified model of F_{bd}, showing a linear relationship between F_{bd} and the maximum electron density of states ($\mathrm{DOS}_{\mathrm{max}}$) within the energy range spanning from the conduction band minimum (CBM) to CBM + E_{g}. Using the Wannier interpolation technique to reduce the cost of calculating the F_{bd} for various three- and two-dimensional materials, we find that the calculated F_{bd} did not show any simple relationship with band gap, but it behaves linearly with the $\mathrm{DOS}_{\mathrm{max}}$, consistent with our theoretical derivation. Our work shows that the $\mathrm{DOS}_{\mathrm{max}}$ is more fundamental than the band gap value in determining the F_{bd}, thus providing useful physical insights into the intrinsic dielectric breakdown strength and opening directions for improving high-power devices. The dimensional effects on F_{bd} has also been revealed that monolayers tend to have larger F_{bd} due to reduced screening effects.

Introduction

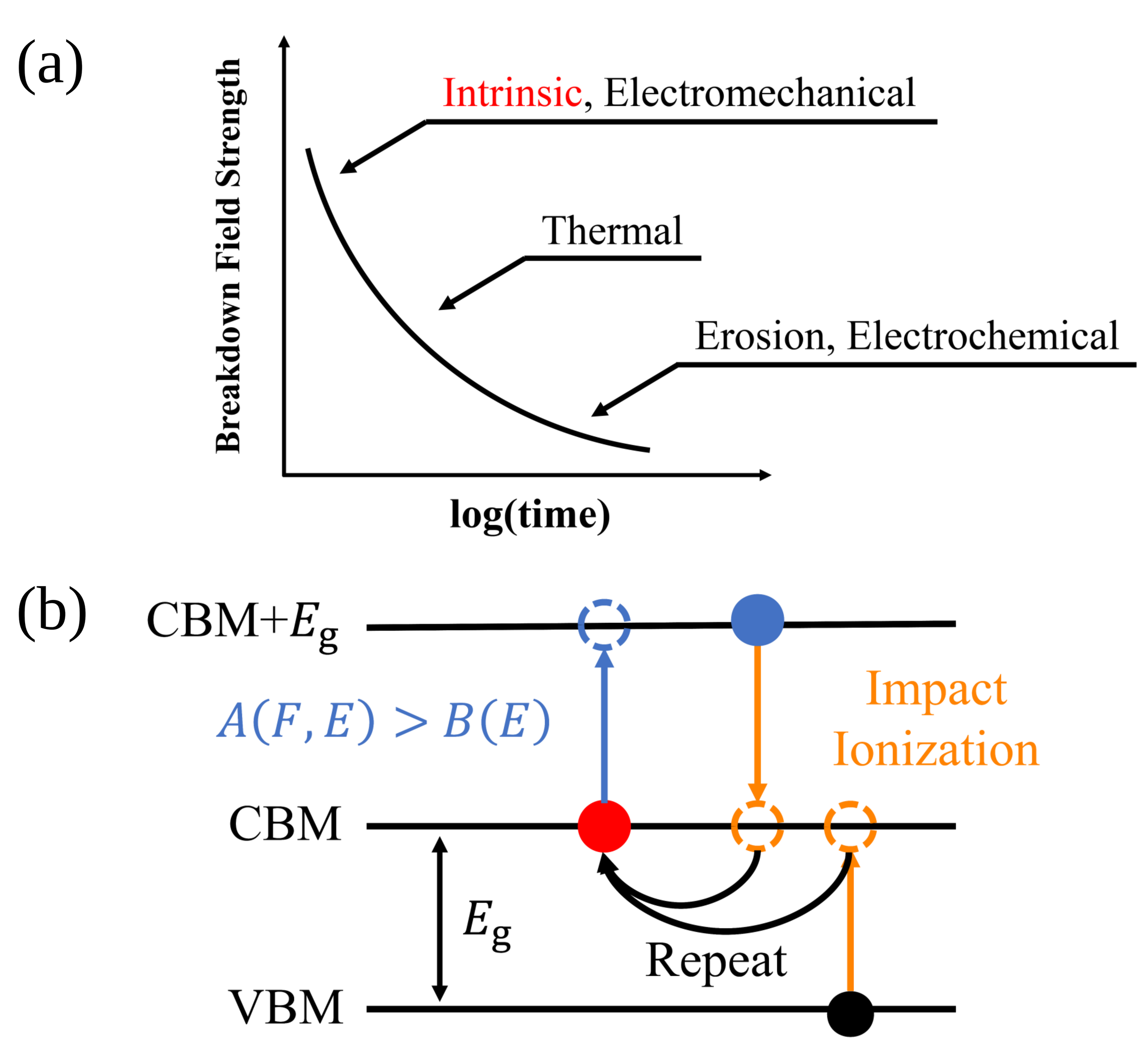

Fig. 1. (a) Comparison between different breakdown mechanism. (b) Schematic diagram for the process of electron avalanche breakdown.

Relation between F_{bd} and $M\mathrm{DOS}_{\mathrm{max}}$

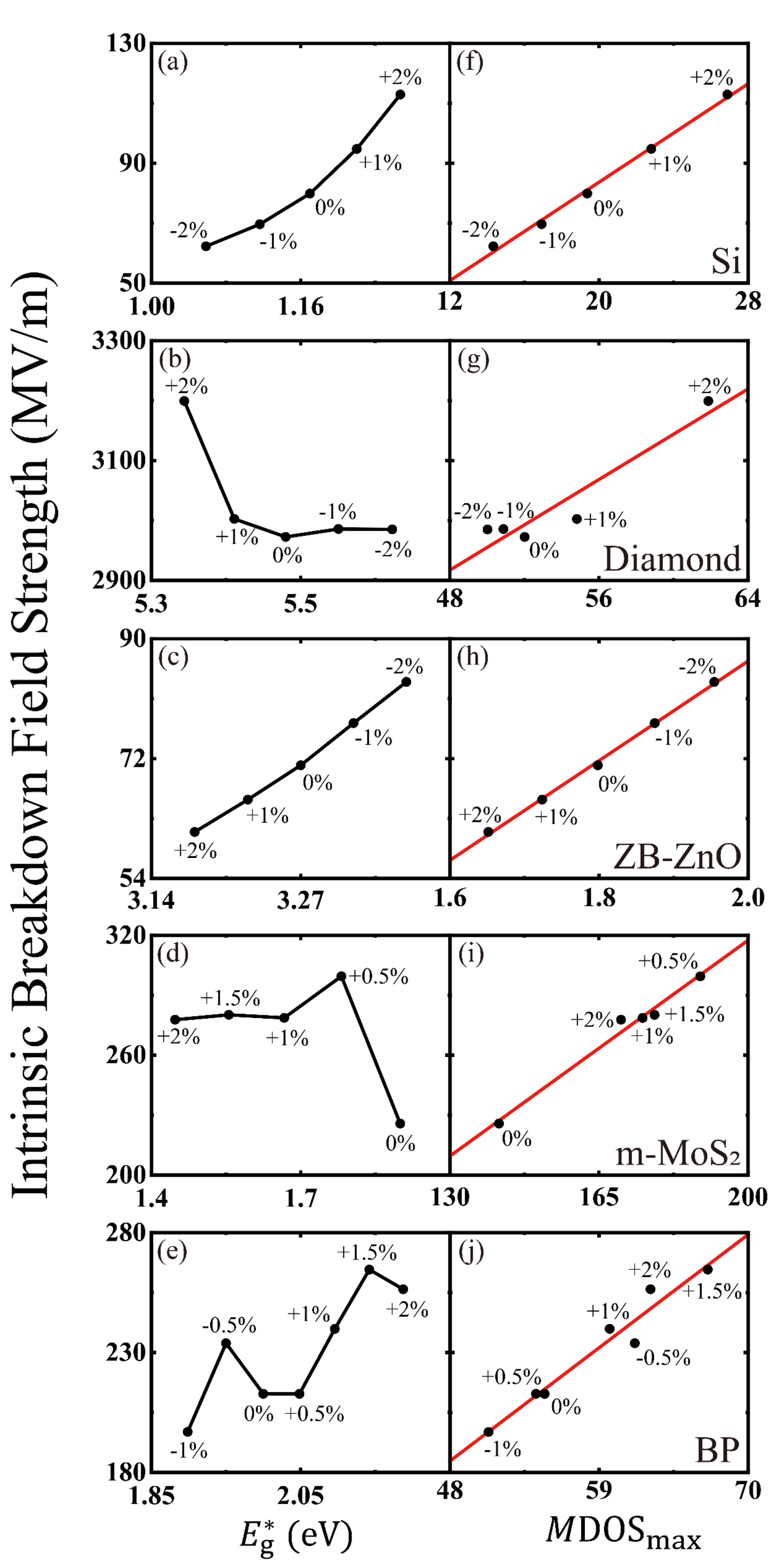

Fig. 2. Comparison of the relation between F_{bd} and band gap with that between F_{bd} and $M\mathrm{DOS}_{\mathrm{max}}$, where $M = \sqrt{m^*\omega_{\mathrm{mean}}}$. Here, the band gap and $\mathrm{DOS}_{\mathrm{max}}$ are tuned using strains, which are labeled for each data.

- The well accepted concept is that a larger band gap often leads to a larger intrinsic breakdown field strength. However, we found that the calculated F_{bd} did not follow a simple relationship with the band gap.
- It is clearly seen from Fig. 2(f)-(j) that F_{bd} is linearly dependent on the normalized $\mathrm{DOS}_{\mathrm{max}}$ for each system, even in cases where the prevailing view does not hold, thus demonstrating our model.

Methods

$$\frac{1}{\tau(E)} = \frac{1}{D(E)}\frac{2\pi}{\hbar}\sum_{\pm}\sum_{n\mathbf{k}}\sum_{\mathbf{q}\nu m}\left|g^{\mathbf{q}\nu}_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}\right|^2\left(n_{\mathbf{q}\nu}+\frac{1}{2}\mp\frac{1}{2}\right) \times \delta\left(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}\pm\hbar\omega_{\mathbf{q}\nu}\right)\delta(\varepsilon_{n\mathbf{k}}-E)$$

$$B(E) = \frac{1}{D(E)}\frac{2\pi}{\hbar}\sum_{\pm}\sum_{n\mathbf{k}}\sum_{\mathbf{q}\nu m}\pm\hbar\omega_{\mathbf{q}\nu}\left|g^{\mathbf{q}\nu}_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}\right|^2\left(n_{\mathbf{q}\nu}+\frac{1}{2}\mp\frac{1}{2}\right) \times \delta\left(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}+\mathbf{q}}\pm\hbar\omega_{\mathbf{q}\nu}\right)\delta(\varepsilon_{n\mathbf{k}}-E)$$

$$F_{\mathrm{bd}} = \mathrm{Max}\left[\frac{\sqrt{3m^*}}{e}\sqrt{\frac{1}{\tau(E)}B(E)}\right], \qquad E \in [\mathrm{CBM}, \mathrm{CBM}+E_{\mathrm{g}}]$$

$$F_{\mathrm{bd}} \approx \frac{\sqrt{3m^*}}{e}\frac{2\pi}{\hbar}g^2_{\mathrm{eff}}\sqrt{(2n_0+1)\hbar\omega_{\mathrm{mean}}}\,\mathrm{DOS}_{\mathrm{max}}$$

$$\mathrm{DOS}_{\mathrm{max}} = \mathrm{Max}[D(E)], \qquad E \in [\mathrm{CBM}, \mathrm{CBM}+E_{\mathrm{g}}]$$

- To reduce the cost of first-principles calculations, we utilized the Wannier interpolation technique.
- We developed an analytical model that shows a linear relationship between F_{bd} and $\mathrm{DOS}_{\mathrm{max}}$ using appropriate approximations.

The calculated breakdown properties

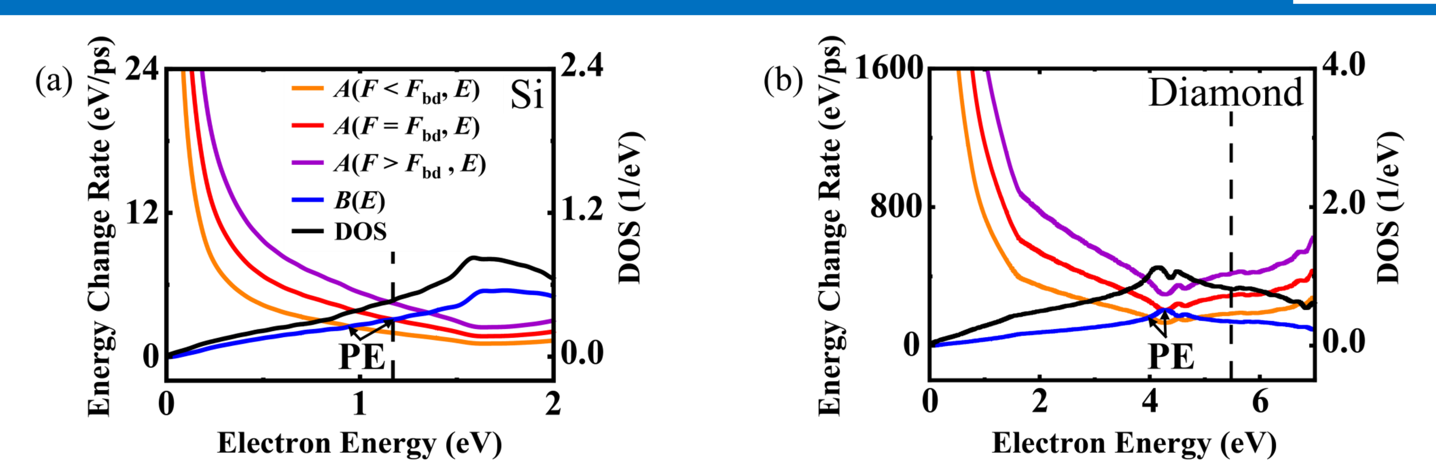

Fig. 3. The calculated energy gain rates, energy loss rates and DOS for (a) Si and (b) diamond.

- The F_{bd} is not directly related to the E_{g} but is determined by the PE maximum, which is governed by the $\mathrm{DOS}_{\mathrm{max}}$.

Conclusion

- We have developed an analytical model that shows a linear relationship between F_{bd} and $\mathrm{DOS}_{\mathrm{max}}$.
- By investigating the behaviors of F_{bd} under different strains in different materials, we show that the $\mathrm{DOS}_{\mathrm{max}}$ is more fundamental than the band gap value in determining the F_{bd}.

References: Y. Sun, S. A. Boggs, and R. Ramprasad, Appl. Phys. Lett. **101**, 132906 (2012). Y. Sun, C. Bealing, S. Boggs, and R. Ramprasad, IEEE Electr. Insul. Mag. **29**, 8 (2013).

S. Liu, H. Xiang, X.-G. Gong, and J.-H. Yang, Phys. Rev. Lett. **134**, 086301 (2025).