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Density of State Models of Steady-State Temperature Dependent Radiation Induced Conductivity

Jodie Corbridge Gillespie and JR Dennison

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Density of States Plots

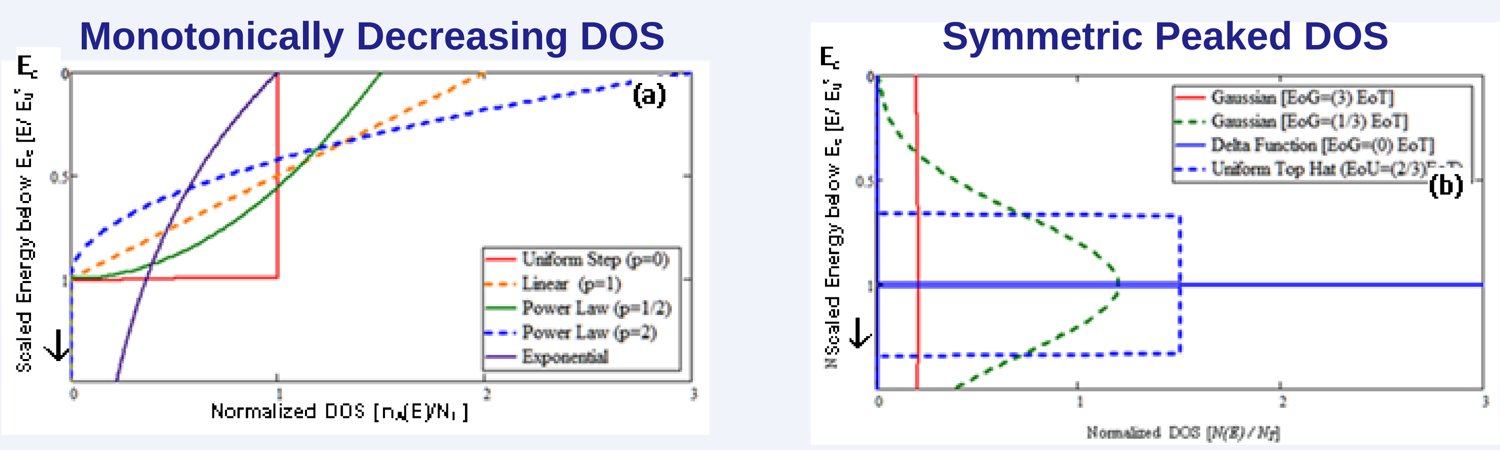

Fig. 1. Density of States (DOS) models. The graphs plot the normalized energy below the conduction band edge as a function of the normalized DOS, $n_A(E) / N_T$. (a) Monotonically decreasing DOS models, including the linear, power law and exponential models, as well as the limiting case uniform model. Power law distributions are shown for two cases, p = ½ < 1 and p = 2 > 1. The energies are normalized by dividing by the width of the distributions, E_o^A. (b) Peaked DOS models, including the Gaussian and delta function models. Gaussian distributions are shown for two cases, (E_o^G/E_o^t) = ⅓ < 1 and (E_o^G/E_o^t) = 3 > 1; the later approaches the limiting case uniform top hat model. The energies are normalized by dividing by the peak of the distributions, E_o^t.

T-Dependent Conductivity Models

DOS Type	Density of Conduction Band Electrons, $n_c(T)$	Temperature Dependence
Monotonically decreasing DOS models with $E_o^t \leq 0$.		
Exponential $0 < E_F^{eff}$	$n_c = (C_o/k_B)DT^{-1/2} \cdot \left\{ \frac{E_o^X}{2k_BT}\left[\left(\frac{N_c}{n_c}\right)^{-\left(\frac{k_BT}{E_o^X}\right)} sinh\left(\frac{2k_BT}{E_o^X}\right) - \frac{2k_BT}{E_o^X}\right]\right\}^{-1}$ $C_o \equiv \frac{\rho_m}{N_T s_c E_{eh} \cdot \sqrt{k_B/m_e}}$	$T^{1/2}$ when $\lvert E_o^X - E_F^{eff}\rvert \gg 2k_BT$
Power Law $0 < E_F^{eff} < E_o^P$	$n_c = \cdot(C_o/k_B)DT^{-1/2} \times \left\{\frac{E_o^P}{4k_BT}\left\{(P_+)^{p+2} - (P_+)(P_-)^{p+1} - \frac{(p+1)}{(p+2)} \cdot [(P_+)^{p+2} - (P_-)^{p+2}]\right\}\right\}^{-1}$ $P_\pm(n_c,T) \equiv \left[1 - \frac{E_F^{eff}(n_c,T)}{E_o^P} \pm \frac{2k_BT}{E_o^P}\right]$	$T^{1/2}$ when $\lvert E_o^P - E_F^{eff}\rvert \gg 2k_BT$
Linear $0 < E_F^{eff} < E_o^L$	$n_c = (C_o/k_B)DT^{-1/2} \cdot \left\{\left[1 - \frac{E_F^{eff}(n_c,T)}{E_o^L}\right]^2 + \frac{1}{3}\left[\frac{2k_BT}{E_o^L}\right]^2\right\}^{-1}$	$T^{-1/2}$ when $\lvert E_o^L - E_F^{eff}\rvert \gg 2k_BT$
Uniform Step $0 < E_F^{eff} < E_o^{US}$	$n_c = (C_o/k_B)DT^{-1/2} \cdot \left[1 - \frac{E_F^{eff}(n_c,T)}{E_o^{US}}\right]^{-1}$	$T^{-1/2}$ when $\lvert E_o^{US} - E_F^{eff}\rvert \gg 2k_BT$
Power Law, Linear,Uniform Step $0 < E_o^A < E_F^{eff-}$ (below distribution)	$n_c = 0$	T-independent
Peaked DOS models with $E_o^t > 0$.		
Gaussian $0 < E_F^{eff}$	$n_c = \cdot(C_o/k_B)DT^{-1/2} \cdot \left[1 + 2 \cdot erf\left(\frac{E_o^G}{\sqrt{2}\,E_{oG}}\right)\right] \times \left\{1 + \left[\frac{\sqrt{2}\,E_o^G)}{2k_BT}\right] \cdot \left[R_+ \cdot erf(R_+) - R_- \cdot erf(R_-) + \frac{\left(e^{-(R_+)^2} - e^{-(R_-)^2}\right)}{\sqrt{2\pi}}\right]\right\}^{-1}$ $R_\pm(n_c,T) \equiv \left\{\frac{\left[E_o^t - E_F^{eff}(n_c,T)\right] \pm 2k_BT}{\sqrt{2}\,E_{E_o^G}}\right\}$	$T^{-1/2}$ when $\left(E_F^{eff} - E_o^t\right) \gg 2k_BT$ (above distribution) $T^{1/2}$ when $\lvert E_o^t - E_F^{eff}\rvert \ll 2k_BT$ (within distribution)
Delta Function $0 < E_F^{eff} < E_o^t$ (above distribution)	$n_c = (C_o/k_B)DT^{-1/2}$	$T^{-1/2}$ when $\lvert E_o^t - E_F^{eff}\rvert \gg 2k_BT$
Delta Function $\lvert E_o^t - E_F^{eff}\rvert \leq 2k_BT$ (within distribution)	$n_c = (C_o/k_B)DT^{-1/2} \cdot \left\{1 + \left[\frac{E_o^t - E_F^{eff}(n_c,T)}{2k_BT}\right]\right\}^{-1}$	$T^{-1/2}$ when $\lvert E_o^t - E_F^{eff}\rvert \ll 2k_BT$
Uniform Top Hat $0 < E_F^{eff} < E_1^U$ (above distribution)	$n_c = (C_o/k_B)DT^{-1/2}$	$T^{-1/2}$ when $\lvert E_o^t - E_F^{eff}\rvert \gg 2k_BT$
Uniform Top Hat $0 < E_1^U < E_F^{eff} < E_2^U$ (within distribution)	$n_c = (C_o/k_B)DT^{-1/2} \cdot \left\{1 - \left[\frac{E_1^{UT} - E_F^{eff}(n_c,T)}{E_o^{UT}}\right]\right\}^{-1}$	$T^{-1/2}$ when $\lvert E_o^t - E_F^{eff}\rvert \gg 2k_BT$
Gaussian, Delta Function, Uniform Top Hat $0 < \left[E_o^t + \frac{1}{2}E_{width\,A}\right] < E_F^{eff-}$ (below distribution)	$n_c = 0$	T-independent

Abstract

Radiation induced conductivity (RIC) occurs when incident radiation deposits energy and excites electrons into the conduction band of insulators. The magnitude of the enhanced conductivity is dependent on a number of factors including temperature and the spatial- and energy-dependence and occupation of the material's distribution of localized trap states within the band gap—or density of states (DOS). Expressions are developed for steady-state RIC over an extended temperature range, based on DOS models for highly disordered insulating materials. A general discussion of the DOS of disordered materials can be given using two simple distributions: one that monotonically decreases below the band edge and one that shows a peak in the distribution within the band gap. Three monotonically decreasing models (exponential, power law, and linear), and two peaked models (Gaussian and delta function) are developed, plus limiting cases with a uniform DOS for each type. Variations using the peaked models are considered, with an effective Fermi level between the conduction mobility edge and the trap DOS, within the peaked trap DOS, and between the trap DOS and the valence band. Explicit solutions, limiting cases, and applications of the models to RIC measurements are presented.

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Calculations

Using the low temperature Fermi-Dirac function approximation from above and assuming $E_F^{eff}(T) \gtrsim 2k_BT$, we can calculate the density of filled trap states, n_t, for the steady-state condition at low T by integrating an expression for the trap state density as a function of energy over all occupied states, or over all trap states in the distribution $n_A(E)$:

$$n_c(T) \approx N_c e^{-E_F^{eff}(T)/k_BT} = \frac{1}{N_T}\int_0^\infty f_{FD}(E,T)\, n_A(E)\, dE \approx$$

$$\frac{1}{N_T}\left\{\int_0^{E_F^{eff-}(T)} n_A(E)dE + \int_{E_F^{eff-}(T)}^{E_F^{eff+}(T)} \frac{1}{2}\left[1 + \frac{E - E_F^{eff}(T)}{2k_BT}\right] n_A(E)dE\right\} \text{where } E_F^{eff\pm}(T) = E_F^{eff}(T) \pm 2k_BT$$

This expression is the only part of the RIC expression that contains information about the material, at least up to a proportionality constant. The second integral in this expression contains all of the temperature dependence of RIC. Inserting this expression into the standard conductivity equations for electron carriers, we arrive at the final expression for temperature dependant RIC:

$$\sigma_{RIC}(T) = k_{RIC}(T)\,\dot{D}^{\Delta(T)} = q_e\,\mu_e\, n_c(T) \approx q_e\mu_e\, C_o\, \dot{D}\; T^{1/2}\left[\int_0^\infty f_{FD}(E,T) f_A(E)dE\right]^{-1}$$

$$\text{with} \quad C_o \equiv \rho_m\left[N_T s_C E_{eh}\sqrt{3k_B/m_e}\right]^{-1}.$$

Table 2 column 2 shows expressions for $n_c(T)$ in the low T approximation, for all DOS listed in Table 1 evaluated with $E_F^{eff}(T)$ below, above, or within $\pm 2k_BT$ of the distributions.

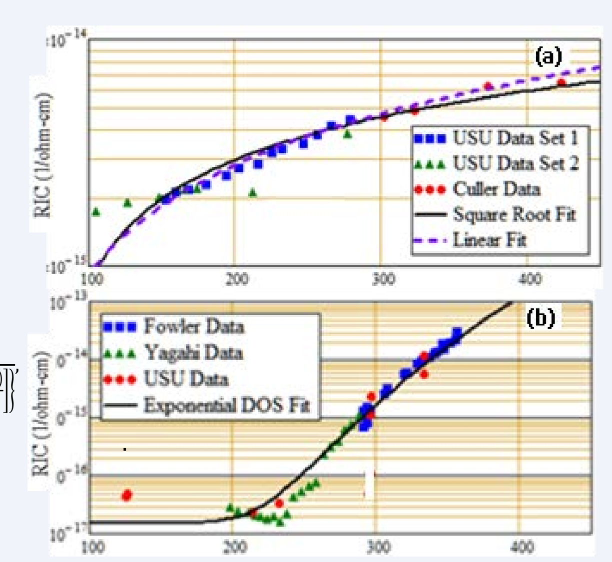
Comparison with Experimental Results

Fig. 3. Radiation induced conductivity versus T for: (a) disordered SiO_2, showing two data sets from USU [3] and Culler [13] with fits proportional to $T^{1.2}$ and T; (b) LDPE, showing data sets from USU [14], Yagahi. [12], and Fowler [6] with a fit based on an exponential DOS. Data from the different studies were scaled to normalize RIC at room T.

$$n_c(T) = \begin{cases} \left[(C_o/k_B)\dot{D}T^{-1/2}\right]^{\left(\frac{T_o^X}{T+T_o^X}\right)}[N_c]^{\left(\frac{T}{T+T_o^X}\right)} \\ ;\ T \to 0\text{ K} \\ \left\{\frac{T}{T_o^X}\right\}\left[(C_o/k_B)\dot{D}T^{-1/2}\right]^{\left(\frac{T_o^X}{T+T_o^X}\right)}[N_c]^{\left(\frac{T}{T+T_o^X}\right)} \\ ;\ E_o^X \equiv k_BT_o^X \gg E_F^{eff}(T) \gtrsim 2k_BT > 0 \end{cases}$$

$$n_c(T) = \frac{(C_o/k_B)\,\dot{D}\,T^{-1/2}\left[1 + 2\cdot erf\left(\frac{E_0^t}{\sqrt{2}E_0^G}\right)\right]}{\left\{1 + \left[\frac{\sqrt{2}\,E_{oG})}{2k_BT}\right]\cdot\left[R_+\cdot erf(R_+) - R_-\cdot erf(R_-) + \frac{\left(e^{-(R_+)^2} - e^{-(R_-)^2}\right)}{\sqrt{2\pi}}\right]\right\}},$$

$$\text{where} \qquad R_\pm(n_c,T) \equiv \left\{\frac{\left[E_o^t - E_F^{eff}(n_c,T)\right] \pm 2k_BT}{\sqrt{2}\,E_{oG}}\right\}$$



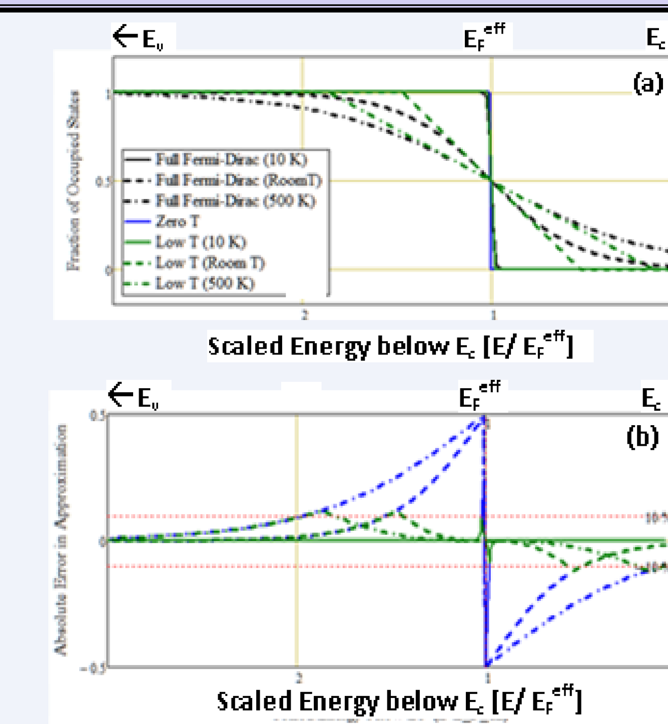
Disordered Silicon Dioxide (SiO_2)

- Fit with a curve proportional to $T^{1.2}$, as would be expected for a material with a peaked DOS with $E_o^t \gg E_F^{eff}(n_c,T) \gg k_BT$.
- Difficult to distinguish over the limited T range whether this is in better agreement than a fit linearly proportional to T.
- USU Data Set 2 shows a smaller decrease in RIC at the lowest T than predicted by either fit; this may have resulted from increased charging during measurements at low T, where conductivity is smallest or may a indicate that the description of the DOS is not exact or other bands are present.
- RIC for SiO_2 increases by only ~4X from ~100-420 K, almost three orders of magnitude less than observed for LDPE over similar T ranges. Cathodoluminescence for these SiO_2 materials have suggested the presence of fairly narrow (~10-50 meV wide) deep level trap DOS distributions within the bandgap [15].

Low Density Polyethylene (LDPE)

- Fit with a curve predicted for an exponential monotonically decreasing DOS [15].
- At T≤250 K, LDPE data exhibits a modest factor of ~3 increase in RIC. Such an increase at low T is predicted for an exponential monotonically decreasing DOS. However, for expected values of $E_o^X$and N_T, these increases are predicted below ~30-50 K.
- Behavior observed in LDPE may alternately be related to a LDPE structural phase transition seen at between 250 K and 262 K. This structural β phase transition is routinely observed in branched PE, and associated with conformational changes along polymer chains in the interfacial matrix of disordered polymer between nanocrystalline regions in the bulk.
- Changes near ~250 K seen in prior studies of mechanical and thermodynamic properties and in dark current conductivity [14,15], RIC [1,14], and other electronic properties.

Low Temperature Approximation



$$f_{FD}(E,T) = \begin{cases} \left\{1 + exp\left[-\left(E - E_F^{eff}\right)/k_BT\right]\right\}^{-1} & ;\quad \text{exact, all } T \\ \Theta\left(E - E_F^{eff}\right) & ;\quad T = 0\text{ K} \\ \begin{vmatrix} 0, \quad \text{if } \left(E - E_F^{eff}\right) < 2k_BT \\ \frac{1}{2}\left\{1 + \left[\left(E - E_F^{eff}\right)/2k_BT\right]\right\}, \text{otherwise} \\ 1, \quad \text{if } \left(E - E_F^{eff}\right) > 2k_BT \end{vmatrix} & ;\quad \text{low T} \\ exp\left[\left(E - E_F^{eff}\right)/k_BT\right] & ;\quad \text{high T} \end{cases}$$

Fig. 2. Fermi Dirac distribution function approximations. (a) Fraction of occupied states versus a scaled energy, $[E/E_F^{eff}(T)]$ from E_C≡0 to $3 \cdot E_F^{eff}$≡0.3 eV at three temperatures: (i) a low temperature, 10 K, which is below typical spacecraft operating environments and temperatures at which RIC is measured; (ii) room temperature; and (iii) a high temperature, 500 K, above which most polymeric materials melt or disassociate an few spacecraft operate. (b) Absolute error versus scaled energy, for the zero and low T approximations. The relative error peaks at ~11% at $\pm[2k_BT/E_F^{eff}(T)]$, independent of T.

Density of States (DOS) Models

DOS Type	Normalized DOS Function, $n_A(E)$	Width, E_o^A [a]	Centroid, $E_{centroid}$ [b]	Fraction of Occupied Traps, f_{A0} [c]
Monotonically decreasing DOS models with $E_o^t \leq 0$.				
Exponential	$n_X(E;E_o^X) = N_T\left[\frac{1}{e \cdot E_o^X}\right] \exp\left(\frac{E_o^X - E}{E_o^X}\right)\Theta(E)$	E_o^X $\left(\frac{1}{e}\text{ width}\right)$	$E_o^X \equiv k_BT_o^X$	$\exp\left(\frac{-E_F^{eff}}{E_o^X}\right)$
Power Law	$n_p(E;E_o^p) = N_T\left[\frac{(p+1)}{E_o^p}\left(\frac{E_o^p - E}{E_o^p}\right)^p\right]\Theta(E_o^p - E)\,\Theta(E)$	E_o^p	$\left(\frac{1}{p+2}\right)E_o^p$	$\left(\frac{E_o^p - E_F^{eff}}{E_o^p}\right)^{(p+1)}$
Linear (Power Law, p = 1)	$n_L(E;E_o^L) = N_T\left[\frac{2}{E_o^L}\left(\frac{E_o^L - E}{E_o^L}\right)\right]\Theta(E_o^L - E)\,\Theta(E)$	E_o^L	$\left(\frac{1}{3}\right)E_o^L$	$\left(\frac{E_o^L - E_F^{eff}}{E_o^L}\right)^2$
Uniform Step (Limit of Top Hat, $E_1^U \to 0$) (Limit of Power Law, p = 0)	$n_{US}(E;E_o^U) = N_T\left[\frac{1}{E_o^U}\right]\Theta(E_o^U - E)\,\Theta(E)$	E_o^U	$\frac{1}{2}E_o^U$	$\left(\frac{E_o^U - E_F^{eff}}{E_o^U}\right)$
Peaked DOS models with $E_o^t > 0$.				
Gaussian	$n_G(E;E_o^G,E_o^t) =$ $N_T\left[1 + 2erf\left(\frac{E_o^t}{\sqrt{2}\cdot E_o^G}\right)\right]^{-1}\left[\frac{2}{\sqrt{2\pi}\cdot E_o^G}\right]\exp\left[-\frac{1}{2}\left[\frac{\lvert E_o^t - E\rvert}{E_o^G}\right]^2\right]\Theta(E)$	$2E_o^G$ (2X Standard Deviation)	Centroid: $E_o^t + \frac{2}{\sqrt{2\pi}\cdot E_o^G}\left\{\frac{e^{-\frac{1}{2}\left(E_o^t/E_o^G\right)^2}}{\left[1 + erf\left(\frac{E_o^t}{\sqrt{2}\cdot E_o^G}\right)\right]}\right\}$ Mean Energy: $\left[1 + 2erf\left(\frac{E_o^t - E_F^{eff}}{\sqrt{2}\cdot E_o^G}\right)\right] / \left[1 + 2erf\left(\frac{E_o^t}{\sqrt{2}\cdot E_o^G}\right)\right]$	
Delta Function (Limit of Gaussian, $E_o^G \to \infty$)	$n_\delta(E;E_o^t) = N_T\;\delta(E_o^t - E)$	$E_o^G \to 0$	E_o^t	1
Uniform Top Hat (Limit of Constant) (Limit of Gaussian, $E_o^G \to \infty$)	$n_{UT}(E;E_1^U,E_2^U) = N_T\left[\frac{1}{E_2^U - E_1^U}\right]\Theta(E_2^U - E)\,\Theta(E - E_1^U)$	$E_o^G \to \infty$ $E_o^U \equiv E_2^U - E_1^U$	$E_o^t = \frac{1}{2}(E_2^U + E_1^U)$	$\left(\frac{E_o^U - E_F^{eff}}{E_o^U}\right)$

$\Theta(E)$ is a Heaviside step function, equal to 0 at $E < 0$ and 1 at $E > 0$.
$\delta(E)$ is the Dirac delta function, equal to infinity at E and zero elsewhere.
$erf(E)$ is the error function evaluated at E.

[a] From Eq. (6).
[b] Mean energy of trap state within band gap, Eq. (2)
[c] From Eq. (7).

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