



# TERAHERTZ MODELING AND SIMULATION

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# Overview



- **AFRL Modeling and Simulation Background**
- **Previous Work**
- **Model Development**
- **Results**
- **Future Considerations**



# Introduction



- **The Air Force Research Laboratory at Brooks City-Base has been a leader in the effort to determine the bioeffects and establish safety standards for **radio frequency and laser energy** for over 20 years**
- **Modeling and Simulation (M&S) expertise above and below the THz region may be leveraged in order to predict potential Bioeffects in the THz region**



# Modeling Procedures



RF-Approach  
THz Modeling

**Skin Model**

**FDTD**

**SAR**

**Pennes Bioheat Solver**

**Thermal Effects**

Laser-Approach  
THz Modeling

**Skin Model**

**Absorption Term**

**Pennes Bioheat Solver**

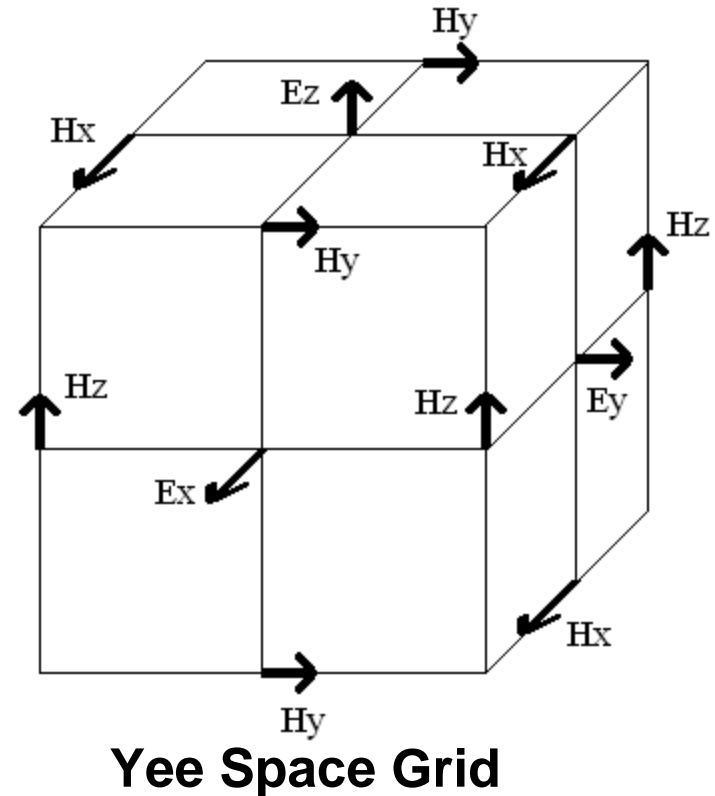
**Thermal Effects**



# Finite Difference Time Domain



- The Finite Difference Time Domain (FDTD) method is a direct time-domain numerical solution technique for Maxwell's equations
  - Yee's algorithm numerically solves for both the Electric and Magnetic fields in a region of interest and over a finite period of time
  - FDTD for electromagnetics was first introduced by Kane Yee in 1966
- Early application for FDTD techniques was scattering problems, e.g., radar cross sections
- As available computational resources increased, FDTD methods became feasible for many classes of problems, including RF dosimetry





# Maxwell's Equations



$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

$$\nabla \cdot \mathbf{D} = \rho_v$$

$$\nabla \cdot \mathbf{B} = 0$$

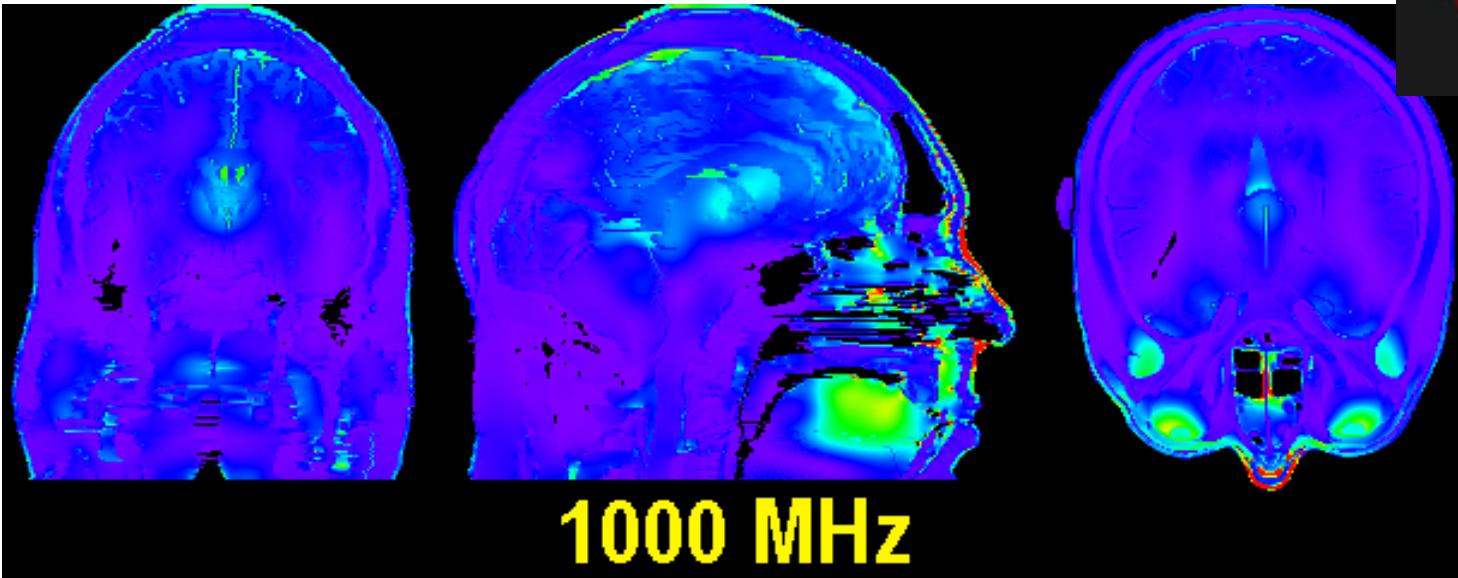
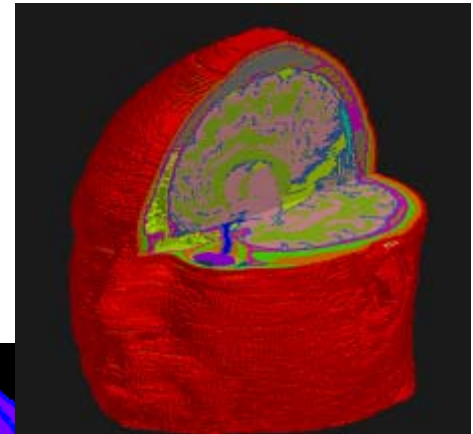




# Previous M&S Work



## Modeling using FDTD (model of absorption of RF energy)

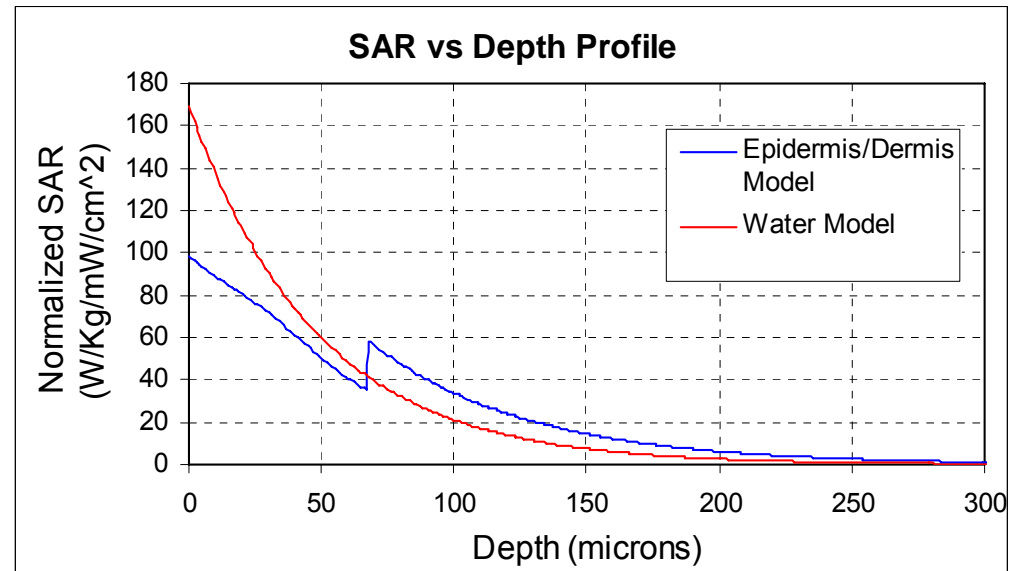




# FDTD Models for THz Energy



- 1D and 2D FDTD codes are used to calculate energy absorption in skin models due to THz energy
- Resolution of skin models is typically set to 1 micron
- Both homogeneous and multi-layer skin slab models are utilized within the FDTD simulations
- Resulting SAR values then serve as input to thermal modeling software



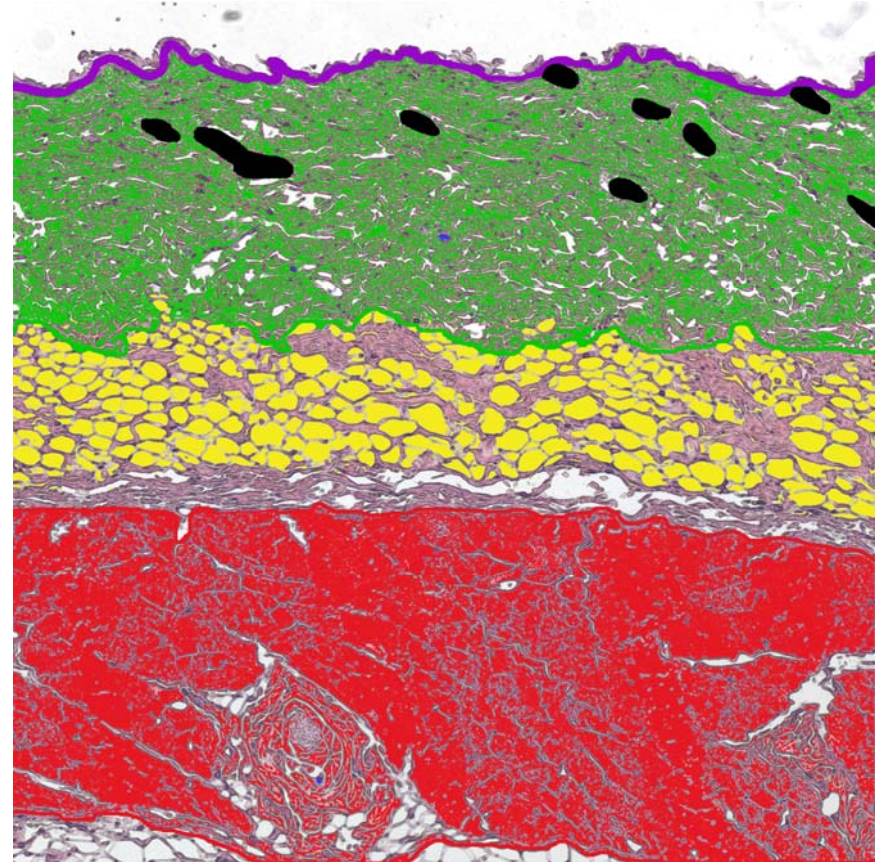
SAR vs. Depth profiles for a uniform 1 THz beam incident upon a water model and a two layer skin model



# FDTD Assumptions and Considerations



- **Compare Modeling and Simulation results to empirical studies**
- **Improved skin models**
  - Realistic skin slab models
  - Further study and refinement of the thermal and electromagnetic properties of skin





# THRESHOLD MODELING RESULTS



- **Thermal Damage Thresholds Modeled**
- **Pulse Duration Ranges for Pure Thermal Effects**
  - Short Pulse (< ~10 microseconds) Work May Require Additional Mechanisms
- **Study Provides Baseline for Injury Threshold Estimates in 0.2 – 2.0 THz Region**
- **Assist in Bridging Exposure Limits (Laser and RF)**
- **Related Laser Research (Strong Absorption) Should Mimic Trends in Damage Thresholds**

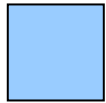
**“THz Frequency Bioeffects,” Draft for RFR Dosimetry Handbook**



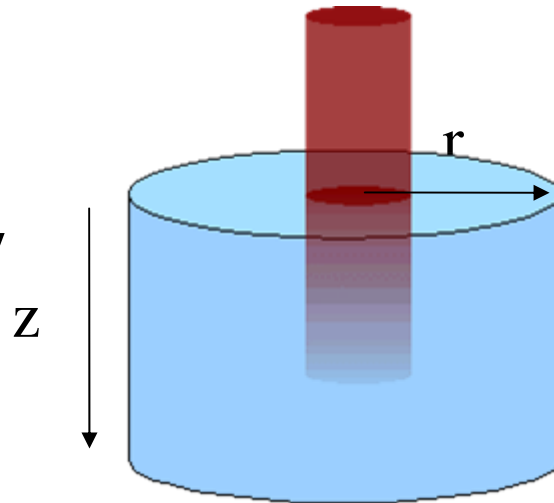
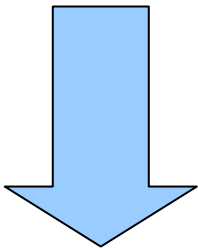
# Our Approach to Heat Transfer



$$\rho c \frac{\partial v}{\partial t} = \nabla \cdot (\kappa \nabla v) + A_I + A_E$$



Cylindrical Symmetry



$$A_I(z, r; t) = \gamma c (T_b - T)$$

$$A_E(z, r; t) = \mu_a I(r, z; t)$$

$$\begin{aligned} \rho(z)c(z) \frac{\partial v(z, r; t)}{\partial t} &= \frac{\kappa(z)}{r} \frac{\partial v(z, r; t)}{\partial r} + \frac{\partial}{\partial r} \left( \kappa(z) \frac{\partial v(z, r; t)}{\partial r} \right) \\ &+ \frac{\partial}{\partial z} \left( \kappa(z) \frac{\partial v(z, r; t)}{\partial z} \right) + A_I(z, r; t) + A_E(z, r; t) \end{aligned}$$

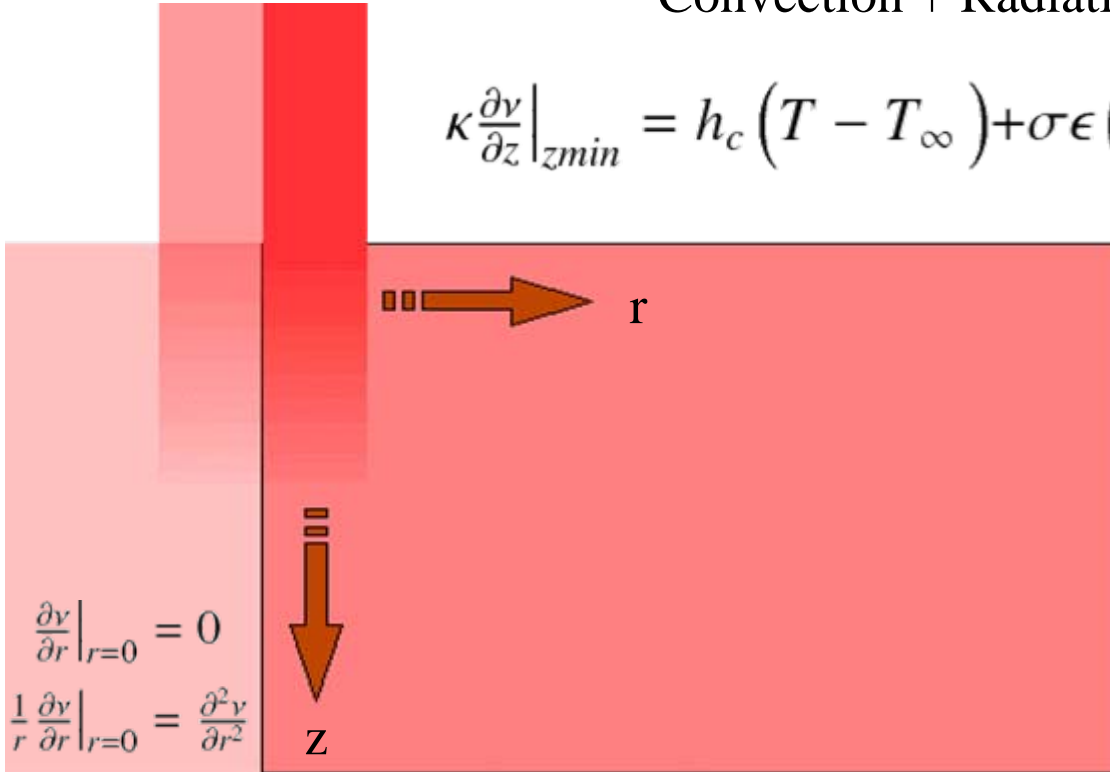


# Complete Boundary Conditions



Convection + Radiative + Evaporative

$$\kappa \frac{\partial v}{\partial z} \Big|_{z_{min}} = h_c (T - T_\infty) + \sigma \epsilon (T^4 - T_\infty^4) + Q_{vap}(T)$$



$$v \Big|_{r_{max}} = 0 \quad \text{Sink / Heat Bath}$$

$$\frac{\partial v}{\partial r} \Big|_{r_{max}} = 0 \quad \text{Insulator}$$

$$-\kappa \frac{\partial v}{\partial z} \Big|_{z_{max}} = h_c (T - T_\infty) + \sigma \epsilon (T^4 - T_\infty^4) + Q_{vap}(T)$$

Convection + Radiative + Evaporative



# Physical Properties

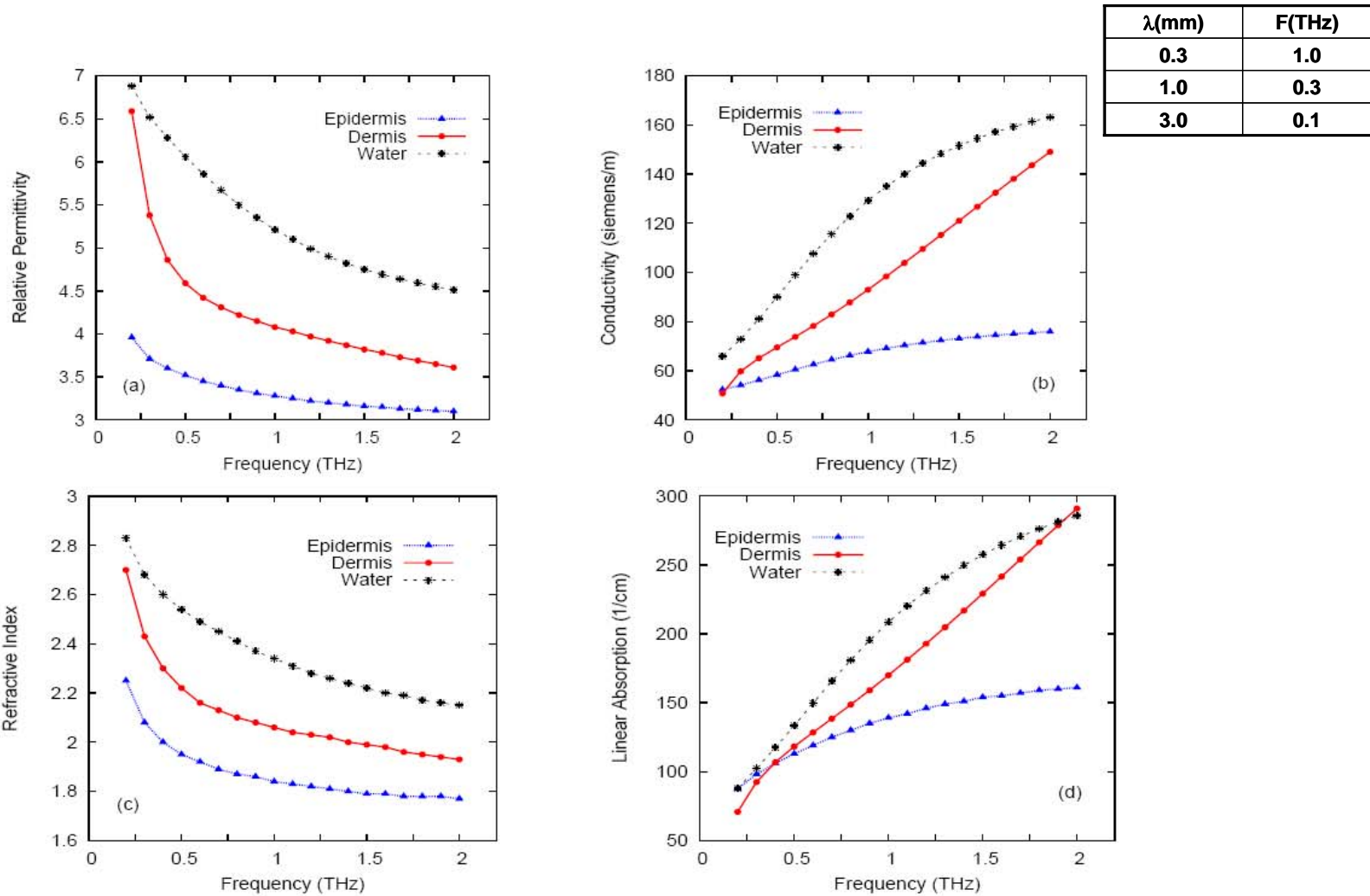


Figure 1: (a) Frequency-dependent permittivity, (b) conductivity, (c) refractive index, and (d) linear absorption values for skin tissues and water.



# Linear Absorption vs. SAR Source Terms

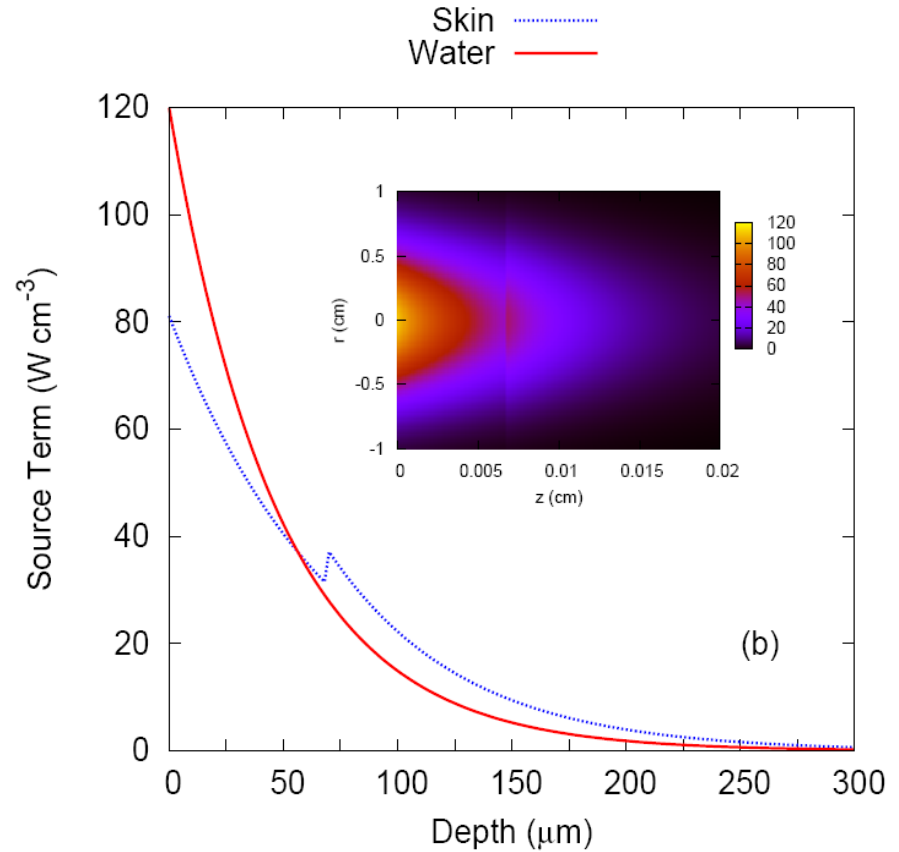
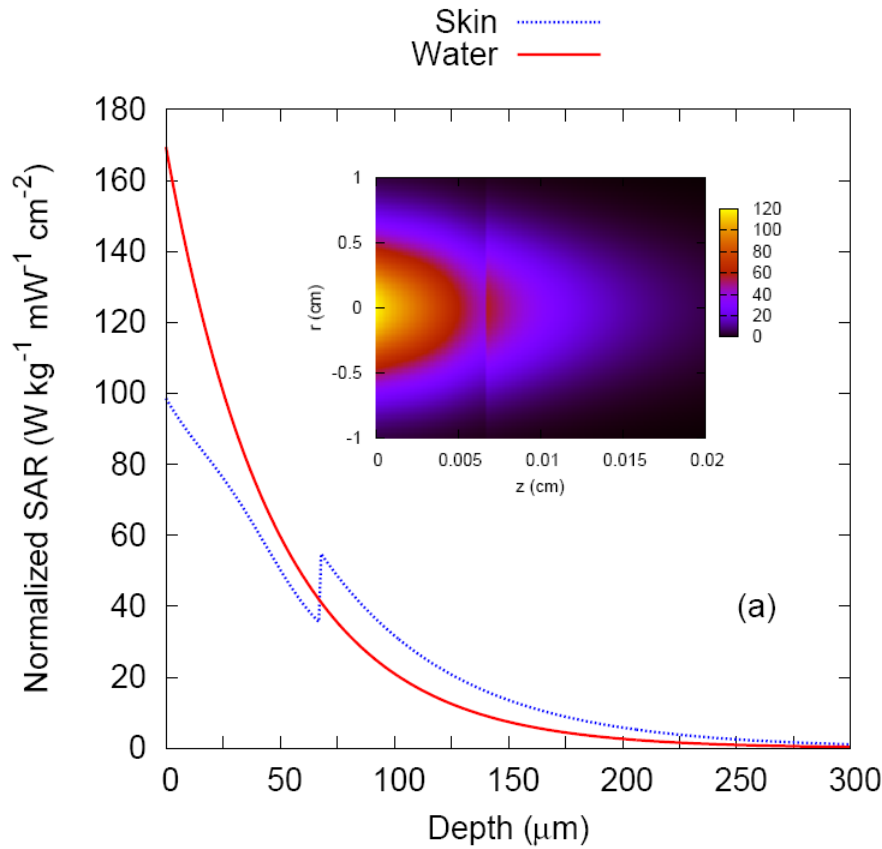


Figure 2: Axial distribution of the source term (a) Normalized SAR (b) Linear Absorption, for two-layer skin model and water for a  $1\text{-W cm}^{-2}$ , 1-THz exposure along  $r = 0$ .



# Ambient Effects Considered

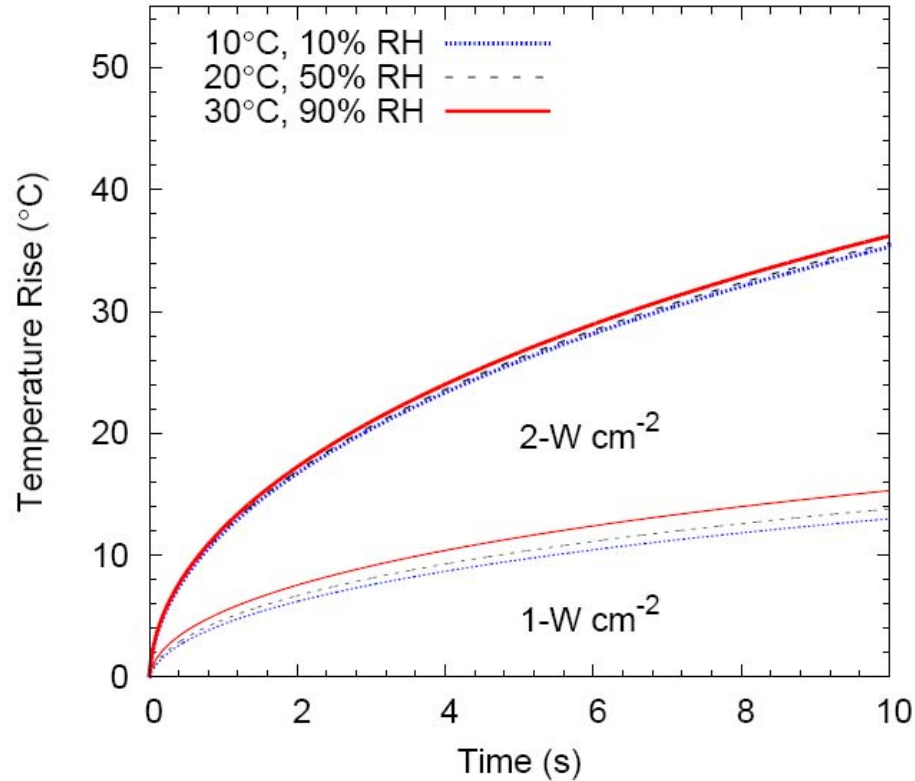


Figure 6: Effect of ambient temperature on maximum surface temperature.



# Thresholds and ANSI (1-mm)

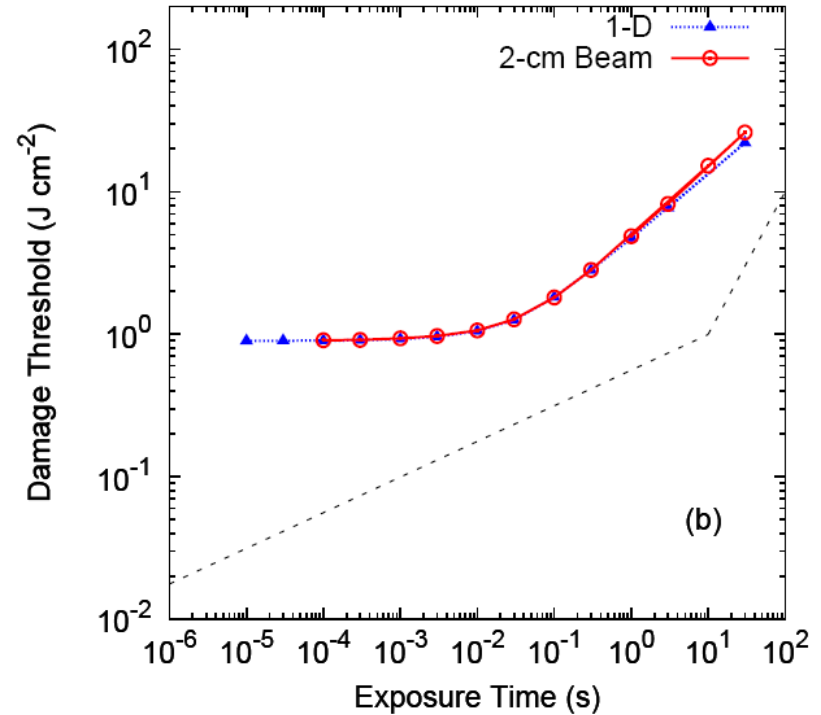
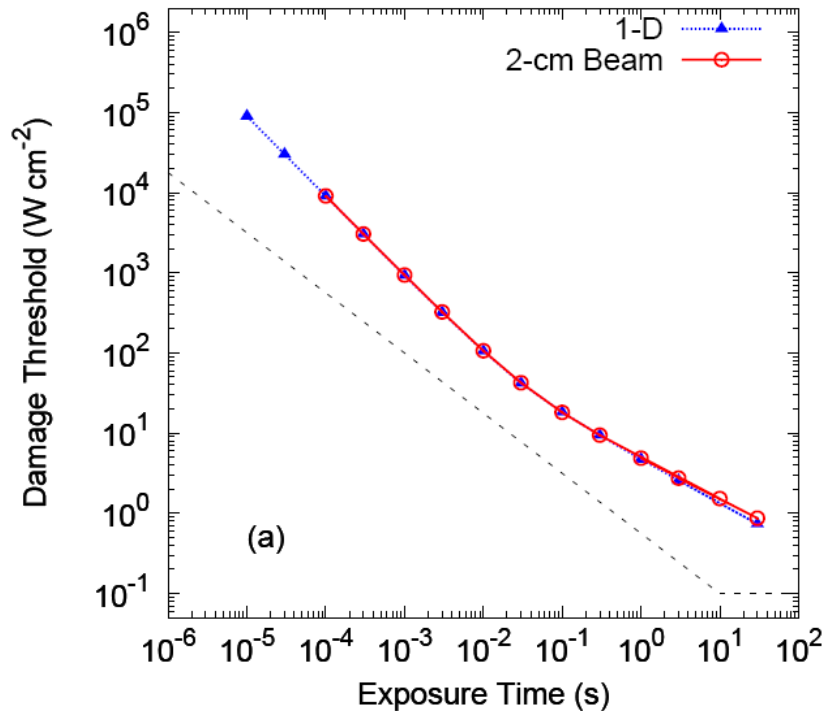


Figure 7: Summary of computed damage thresholds as a function of exposure time for one-dimensional simulations and a 2-D simulation of 2-cm beam diameter (Gaussian distribution), 1-THz exposures. Panel (a) shows the threshold as irradiance ( $W cm^{-2}$ ) and (b) shows the same results as radiant exposure ( $J cm^{-2}$ ).



# Spot Size Dependence of Threshold

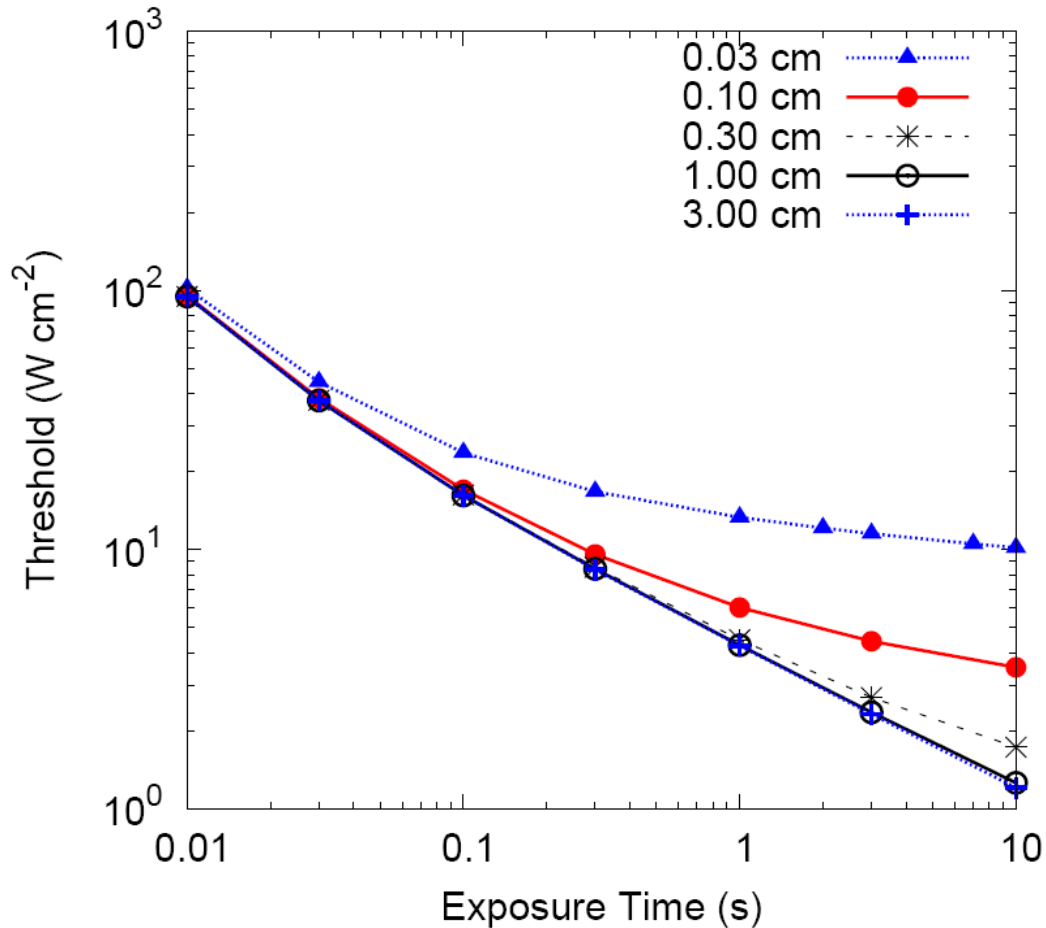


Figure 10: Beam diameter (Gaussian  $e^{-1}$  irradiance point) dependence of damage threshold for differing exposure durations at 1 THz.



# Peak Temperature at Threshold

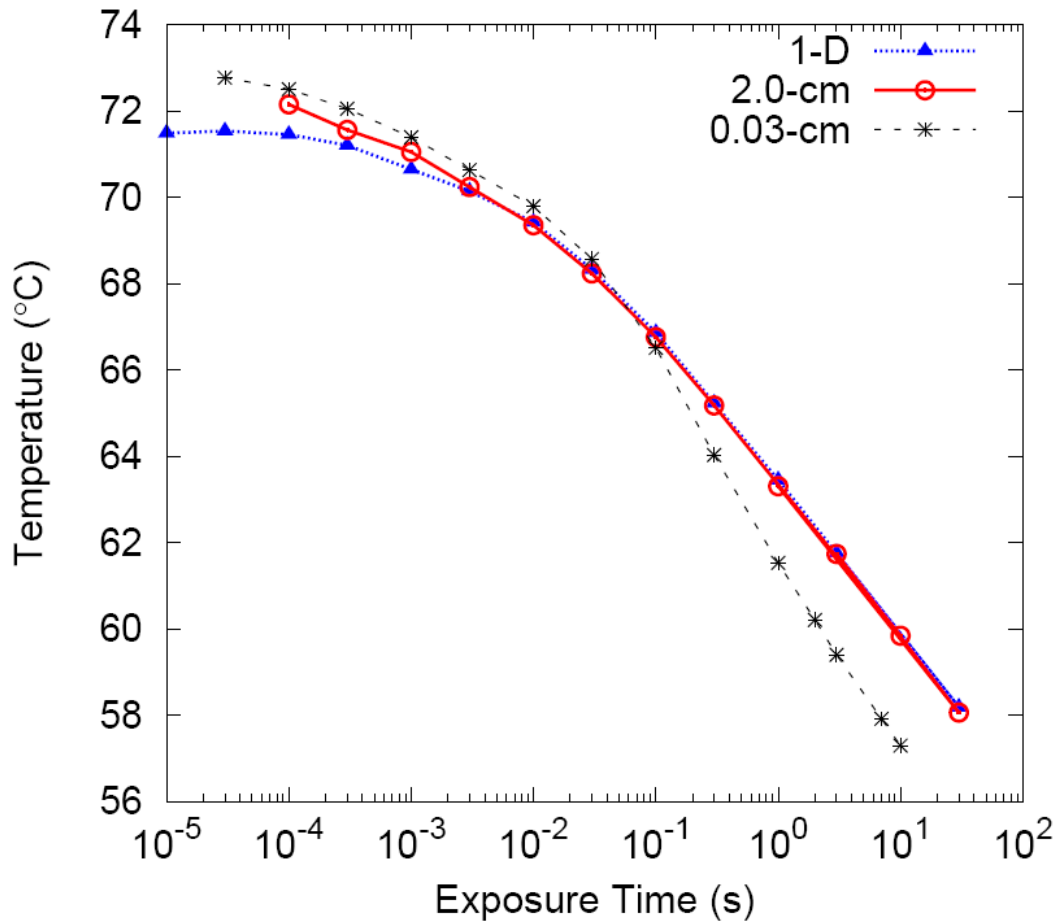
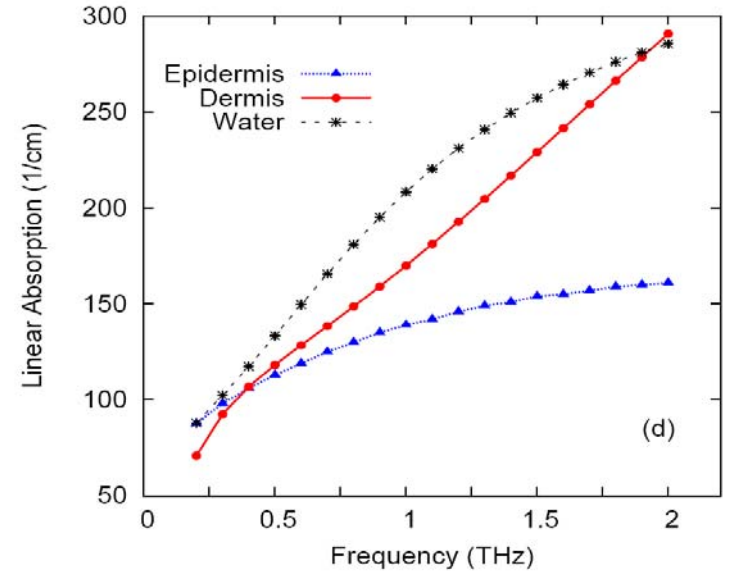
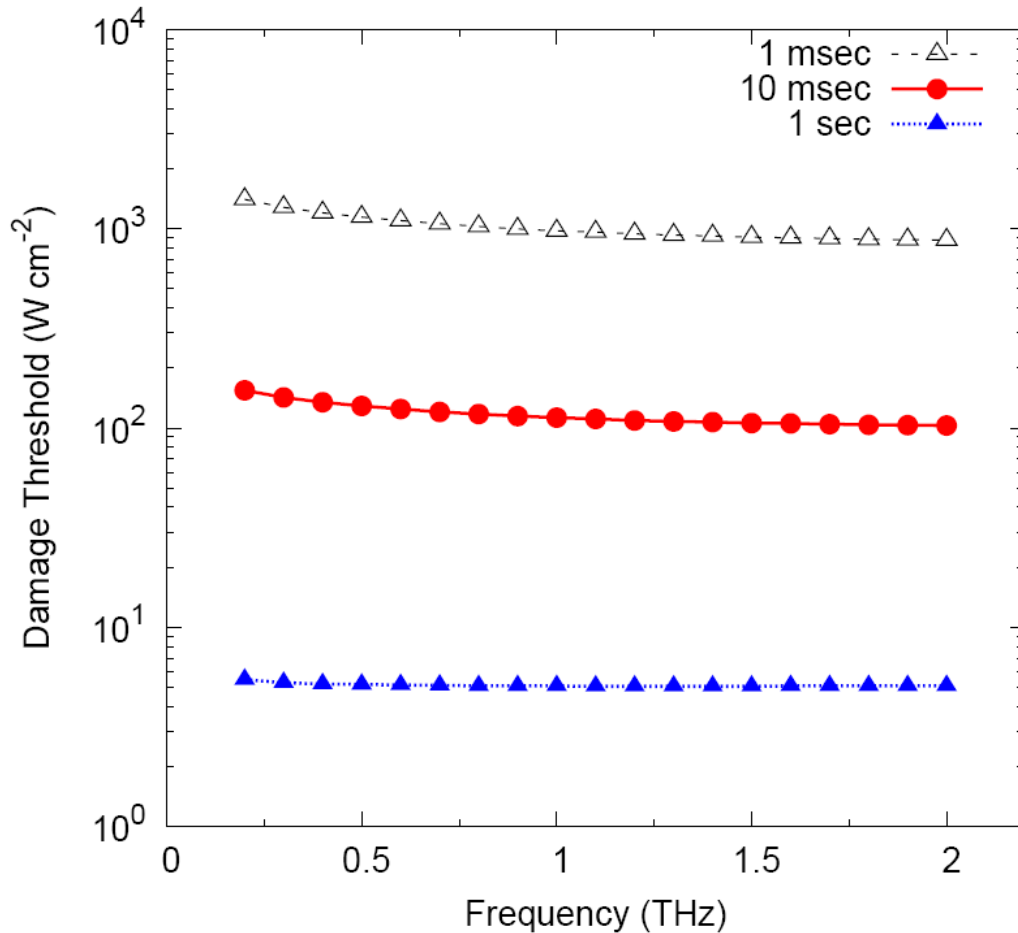


Figure 8: Summary of computed temperature rise at the damage threshold for a number of beam diameter values (Gaussian distribution), 1-THz exposures.



# Frequency-Dependence of Thresholds



$\lambda(\text{mm})$	F(THz)
0.3	1.0
1.0	0.3
3.0	0.1

Figure 11: Frequency dependence of damage thresholds for three differing exposure times for the 1-D linear absorption model.



# Comparison to Expt. Data

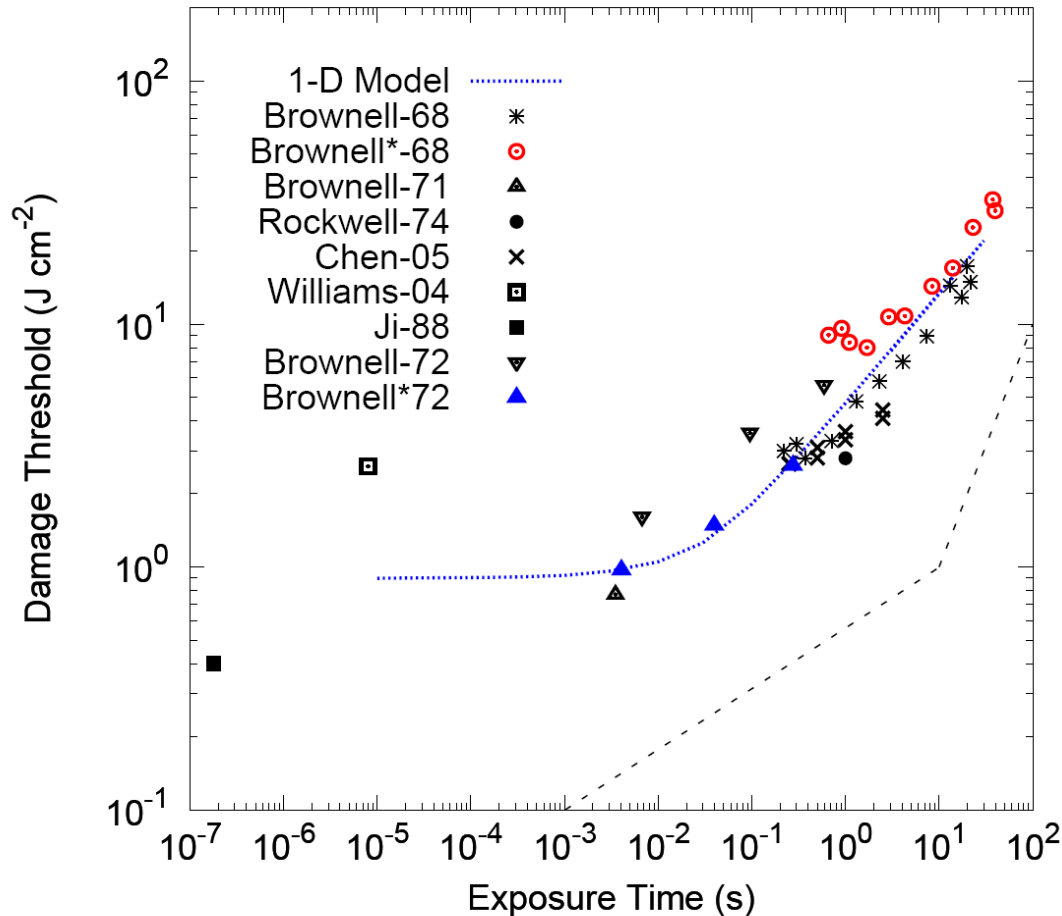
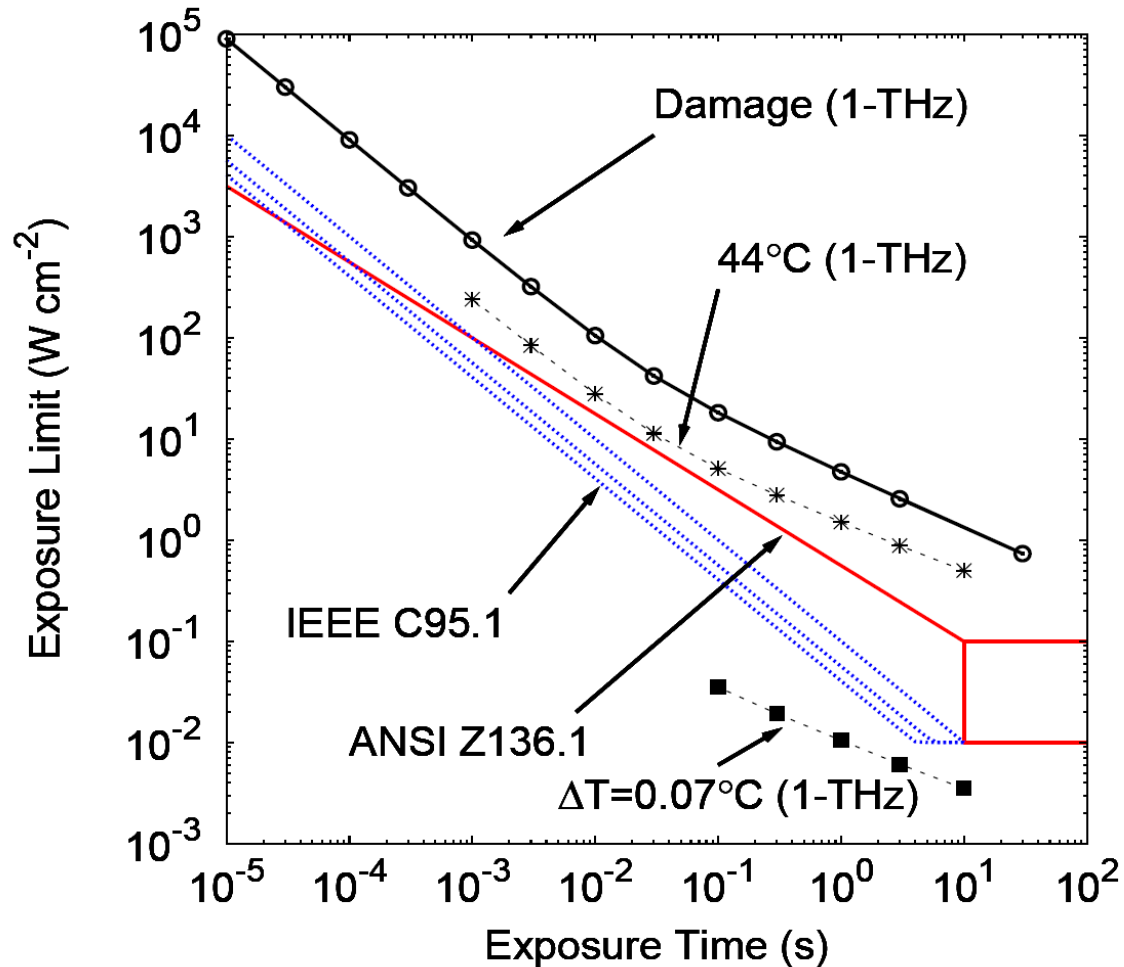


Figure 13: A comparison of 1-THz damage threshold estimates to experimental data from other strongly absorbed wavelengths. Citations marked with an asterisk indicate blistering threshold endpoints. The dashed line in the lower right is the applicable ANSI Z136.1-2000 exposure limit.



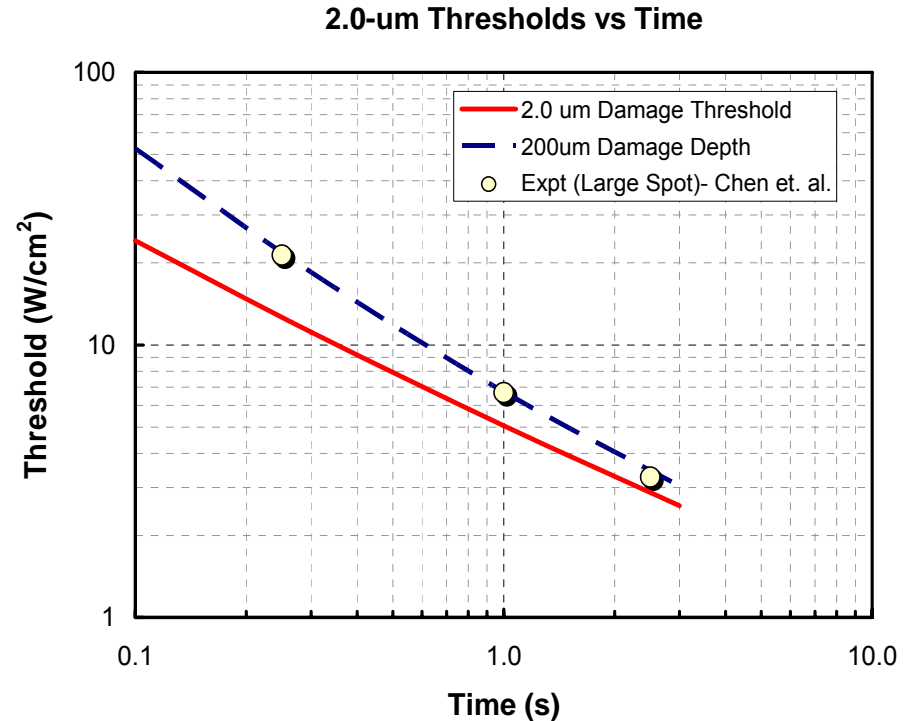
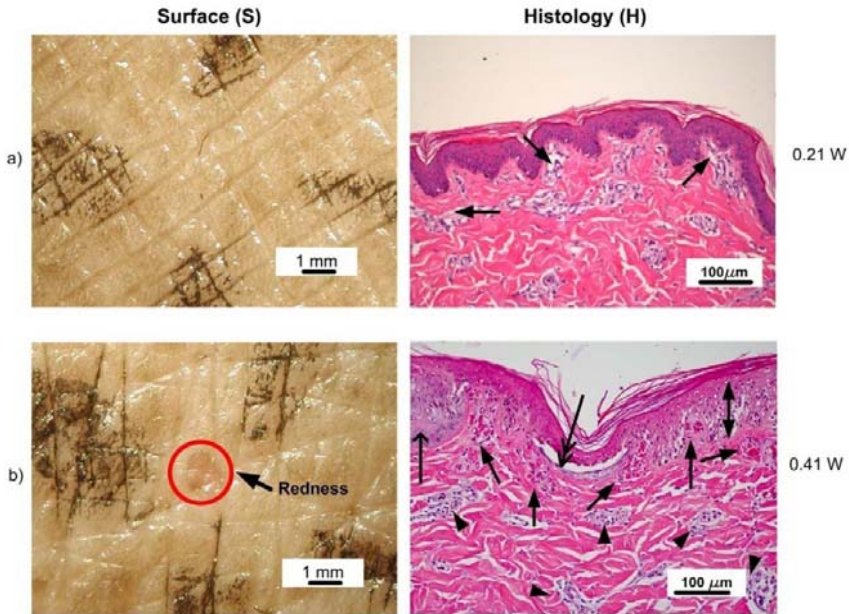
# Standards, Thresholds, and Sensation



A comparison of various thresholds and exposure limits for frequencies near 1 THz



# Food for Further Thought (Study)



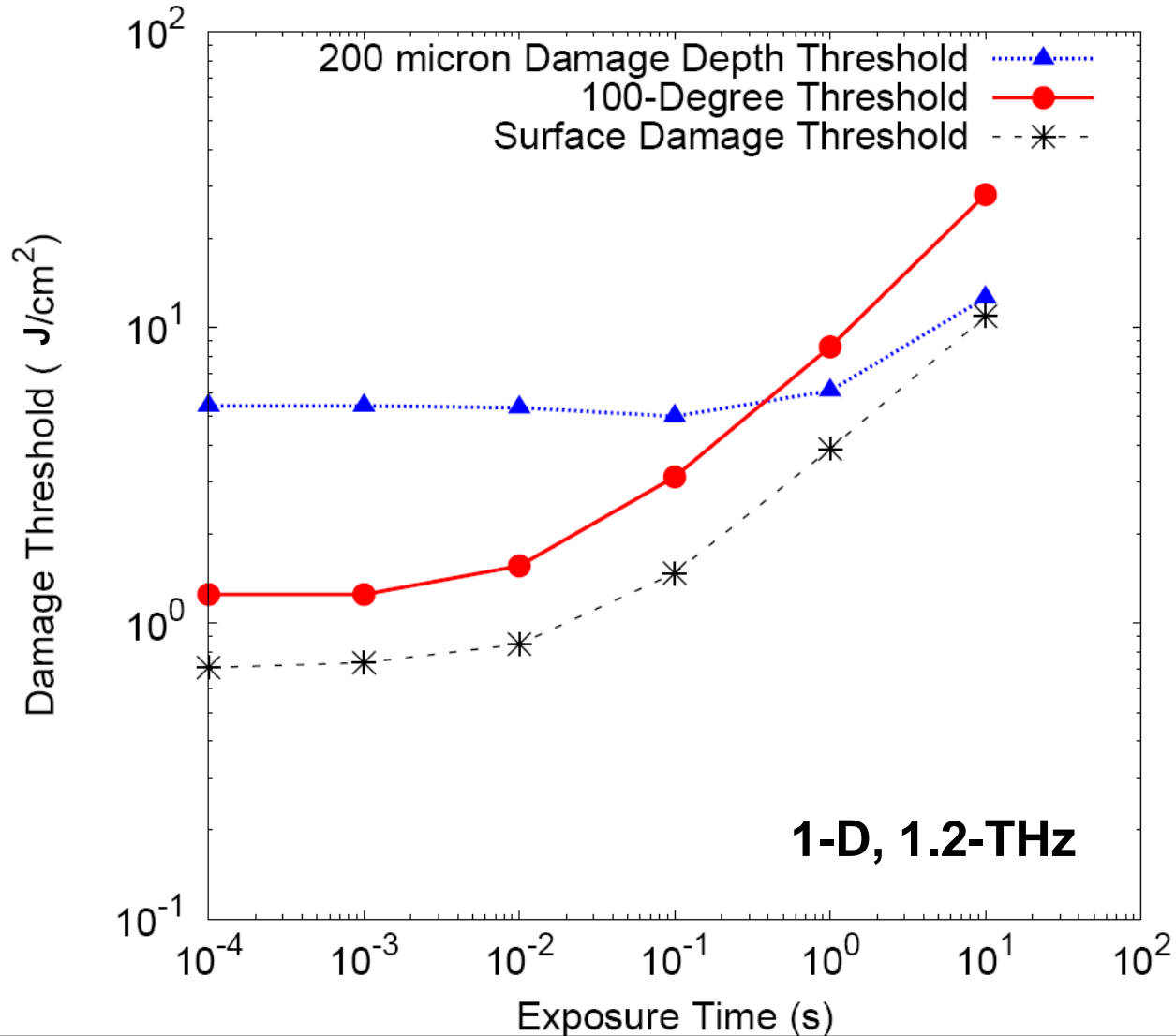
Chen, et. al. Histological and Modeling Study of Skin Thermal Injury to 2.0  $\mu m$  Laser Irradiation *in press Lasers Surg. Med.* (2007).

(and SPIE Photonics West 2007)

**200  $\mu m$  – depth damage at threshold endpoint**



# THz Thermal Damage Implications





# The Whole Story?



- **Thermal Damage Thresholds Only**
- **Estimates from Published Tissue Values**
- **Short-Pulse (non-thermal) Mechanisms Not Addressed**
- **Experimental Validation of Damage Thresholds Needed to Anchor Model (and Assumptions)**
  - **Strongest Validation from Existing Experimental Data at Much Higher Frequencies**
- **Threshold Endpoint Assumptions need Refinement – See Chen et. al., 2.0 micron Histopathology Study, 2007 (In Press)**



# Acknowledgements



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  - **Dr. Pat Roach**
  
- **AFRL/HEDO (AFRL/RHDO)**
  - **Mr. Paul Maseberg**
  - **Mr. C.D. Clark III**



# Selected References



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- **Clark CD, Thomas RJ, Maseberg PDS, Buffington GD, Irvin LJ, Stolarski J, Rockwell BA, Modeling of surface thermodynamics and damage thresholds in the IR and THz regime, in: *Optical Interactions with Tissues and Cells XVIII*, vol. 643505, 1–12, SPIE; 2007.**
- **Taflove A, Hagness SC, *Computational Electrodynamics - The Finite-Difference Time-Domain Method*, 2<sup>nd</sup> ed., Artech House, Norwood, MA; 2000.**
- **Pickwell E, Cole B, Fitzgerald AJ, Wallace V, Pepper M, Simulation of terahertz pulse propagation in biological systems. *Applied Physics Letters* 84:2190–2192; 2004.**
- **Pickwell E, Fitzgerald A, Cole B, Taday P, Pye R, Ha T, Pepper M, Wallace V, Simulating the response of terahertz radiation to basal cell carcinoma using ex vivo spectroscopy measurements. *Journal of Biomedical Optics* 10:064021; 2005.**



- **BACKUP SLIDES**

Ref.	Wave-length [ $\mu m$ ]	$\mu_a$ [ $cm^{-1}$ ]	Beam Dia. [cm]	Exp Time [s]	Damage Thresh [ $J cm^{-2}$ ]	End- Point
(Brownell et al. 1969)	10.6	260	1.9	0.22	3.0	Erythema
(Brownell et al. 1969)	10.6	260	1.9	0.30	3.2	Erythema
(Brownell et al. 1969)	10.6	260	1.9	0.37	2.8	Erythema
(Brownell et al. 1969)	10.6	260	1.9	0.71	3.3	Erythema
(Brownell et al. 1969)	10.6	260	1.9	1.3	4.8	Erythema
(Brownell et al. 1969)	10.6	260	1.9	2.3	5.8	Erythema
(Brownell et al. 1969)	10.6	260	1.9	4.1	7.0	Erythema
(Brownell et al. 1969)	10.6	260	1.9	7.4	8.9	Erythema
(Brownell et al. 1969)	10.6	260	1.4	13.1	14.4	Erythema
(Brownell et al. 1969)	10.6	260	1.4	17.4	12.9	Erythema
(Brownell et al. 1969)	10.6	260	1.4	19.9	17.3	Erythema
(Brownell et al. 1969)	10.6	260	1.4	21.6	14.9	Erythema
(Brownell et al. 1969)	10.6	260	1.9	0.66	9.0	White Burn
(Brownell et al. 1969)	10.6	260	1.9	0.91	9.6	White Burn
(Brownell et al. 1969)	10.6	260	1.9	1.1	8.4	White Burn
(Brownell et al. 1969)	10.6	260	1.9	1.7	8.0	White Burn
(Brownell et al. 1969)	10.6	260	1.9	2.9	10.7	White Burn
(Brownell et al. 1969)	10.6	260	1.9	4.3	10.8	White Burn
(Brownell et al. 1969)	10.6	260	1.4	8.4	14.3	White Burn
(Brownell et al. 1969)	10.6	260	1.4	14.0	17.0	White Burn
(Brownell et al. 1969)	10.6	260	1.4	23.0	25.0	White Burn
(Brownell et al. 1969)	10.6	260	1.4	37.4	32.5	White Burn
(Brownell et al. 1969)	10.6	260	1.4	39.6	29.3	White Burn
(Brownell et al. 1971)	10.6	260	2.0	$3.5 \times 10^{-3}$	0.77	Erythema
(Brownell & Stuck 1972)	10.6	260	1.26	$590 \times 10^{-3}$	5.60	Blister
(Brownell & Stuck 1972)	10.6	260	1.33	$95.4 \times 10^{-3}$	3.57	Blister
(Brownell & Stuck 1972)	10.6	260	0.80	$6.71 \times 10^{-3}$	1.61	Blister
(Brownell & Stuck 1972)	10.6	260	1.26	$275 \times 10^{-3}$	5.60	Erythema
(Brownell & Stuck 1972)	10.6	260	1.33	$39.6 \times 10^{-3}$	3.57	Erythema
(Brownell & Stuck 1972)	10.6	260	0.80	$4.05 \times 10^{-3}$	1.61	Erythema
(Rockwell & Goldman 1974)	10.6	260	1.0	1.0	2.8	Erythema
(Chen et al. 2005)	2.0	20-60	1.1	0.25	2.65	Erythema
(Chen et al. 2005)	2.0	20-60	1.1	0.5	3.10	Erythema
(Chen et al. 2005)	2.0	20-60	1.1	1.0	3.61	Erythema
(Chen et al. 2005)	2.0	20-60	1.1	2.5	4.42	Erythema
(Chen et al. 2005)	2.0	20-60	1.4	0.25	2.67	Erythema
(Chen et al. 2005)	2.0	20-60	1.4	0.5	2.81	Erythema
(Chen et al. 2005)	2.0	20-60	1.4	1.0	3.34	Erythema
(Chen et al. 2005)	2.0	20-60	1.4	2.5	4.09	Erythema
(Ji & Liangshun. 1988)	10.6	260	1.0	$180 \times 10^{-9}$	0.40	Erythema
(Bostick et al. 2005)	3.8	37	2.0	$8.0 \times 10^{-6}$	2.6	Erythema



# Thermal Modeling

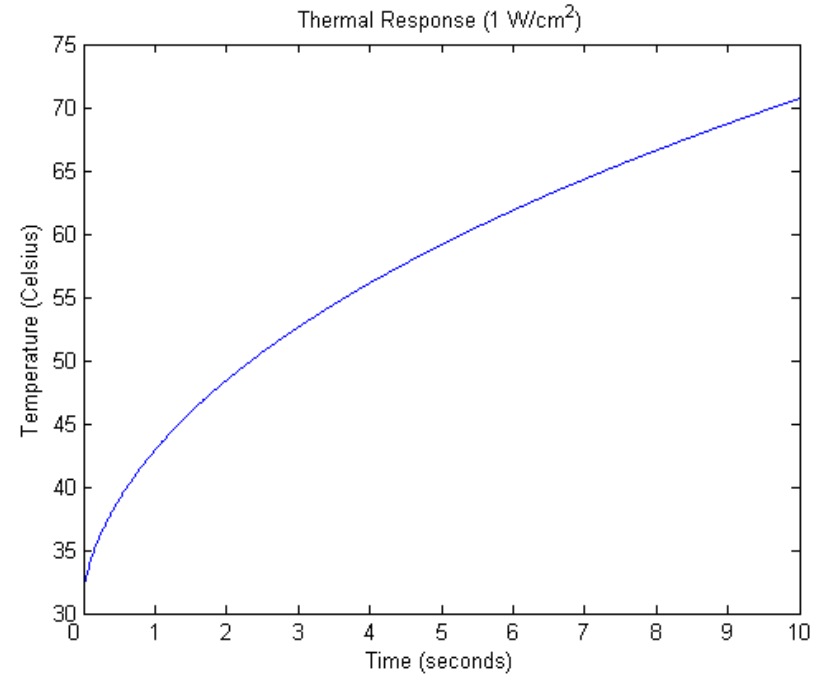


- **Pennes Bioheat solvers are used to predict thermal effects and damage thresholds (2<sup>nd</sup> Degree Burn) within skin slab models**
- **Bioheat equation is modified to take SAR values as thermal input**

$$\rho C \frac{\partial T}{\partial t}(x,t) = \nabla \cdot [k \nabla T(x,t)] + SAR(x,t) \rho - W_b C_b [T(x,t) - T_{art}]$$

- **Arrhenius Integral has been implemented within software to predict damage thresholds for a given exposure condition**

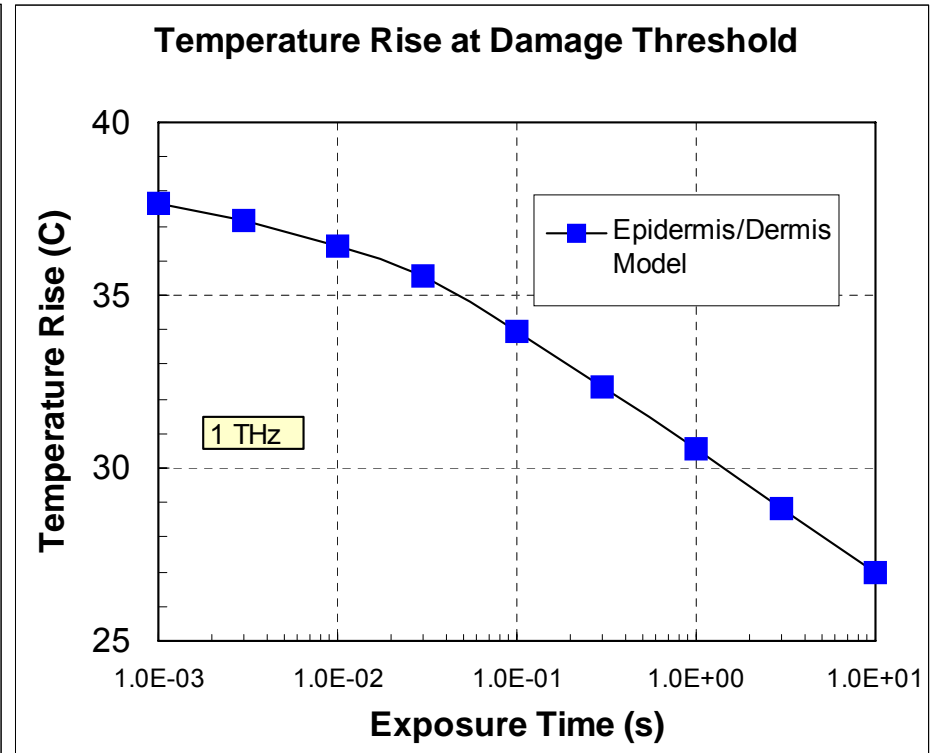
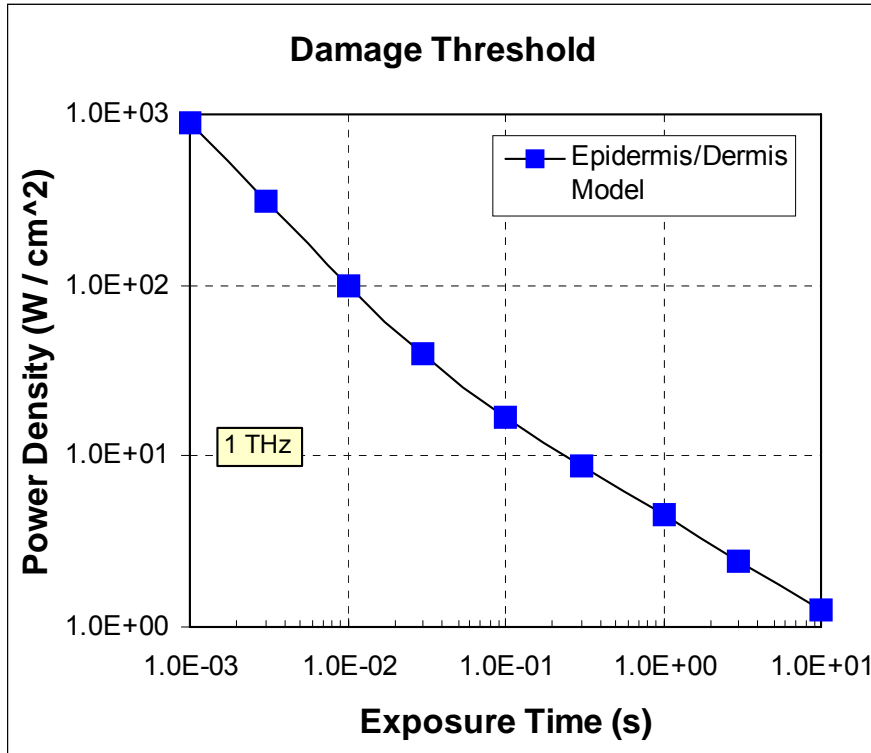
$$\Omega(z) = C \int_{t_1}^{t_2} \exp\left(\frac{-E_a}{RT(z,t)}\right) dt$$



Temperature rise in skin slab model due to a uniform 1 THz beam with incident power density of 1 W / cm<sup>2</sup>



# Thermal Modeling Cont.





# Warmth Detection and Pain Thresholds



- Heating of the skin to 43-46°C has been shown to cause discomfort
- Warmth detection on the skin may occur for a temperature rise of 0.07°C
- Permissible exposure limits adopted for the THz region may take into account such warmth, pain and damage thresholds

