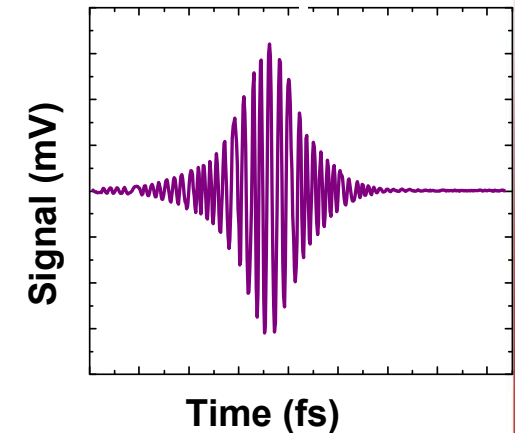
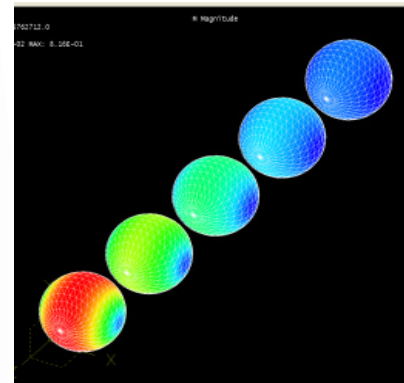
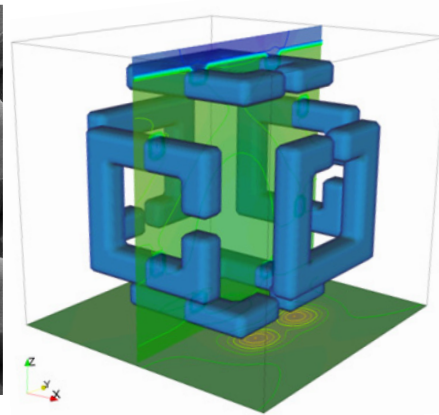
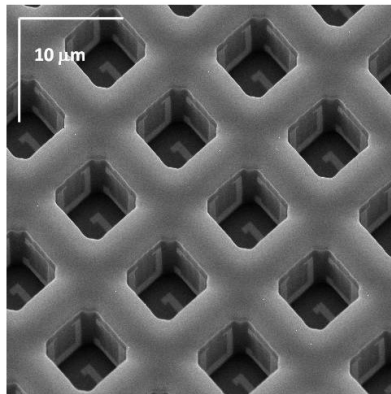


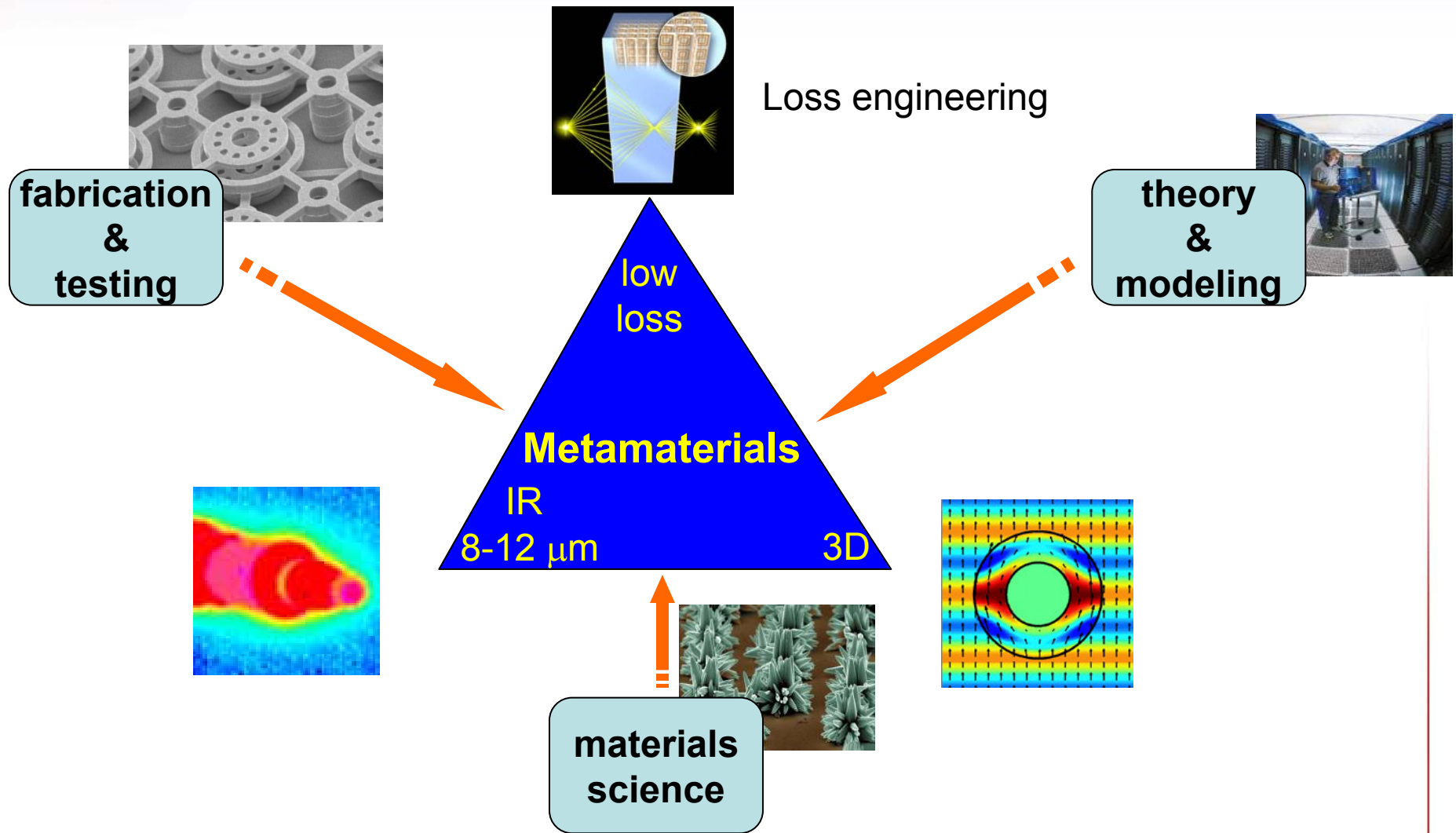
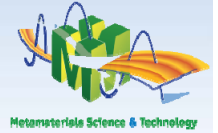
# Metamaterials in the Thermal Infrared

**Michael B. Sinclair**  
**Electronic & Nanostructured Materials Department**  
**Sandia National Laboratories**  
**Albuquerque, NM**



META'10 2/23/2010

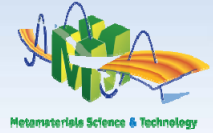
# Sandia's Metamaterial Program





# Sandia's Metamaterial Team

---



**PI: Mike Sinclair**  
**PM: Rick McCormick**

## **Design:**

- Lori Babilio
- Larry Warne
- Dave Peters
- William Langston
- Jacques Loui
- William Johnson

## **Materials:**

- Paul Clem
- Shawn Dirk
- Kamiyar Rahimian
- James Carroll
- Jon Ihlefeld
- Alex Lee

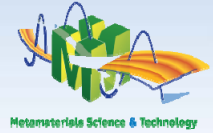
## **Fabrication:**

- Igal Brener
- Bruce Burckel
- Greg Ten-Eyck
- Joel Wendt
- James Ginn
- Eric Shaner
- Brandon Passmore
- Daniel Bender
- Rob Ellis

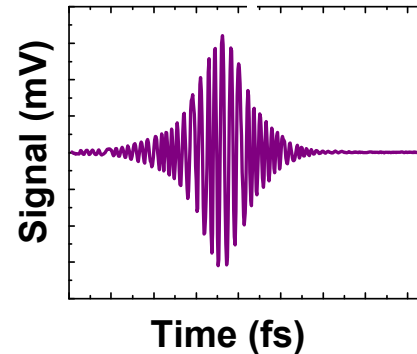
## **Collaborations:**

- Glenn Boreman, UCF/CREOL
- Steve Brueck, UNM
- Ed Kuester, CU Boulder
- Gennady Shvets, UT Austin
- Costas Soukoulis, Iowa State

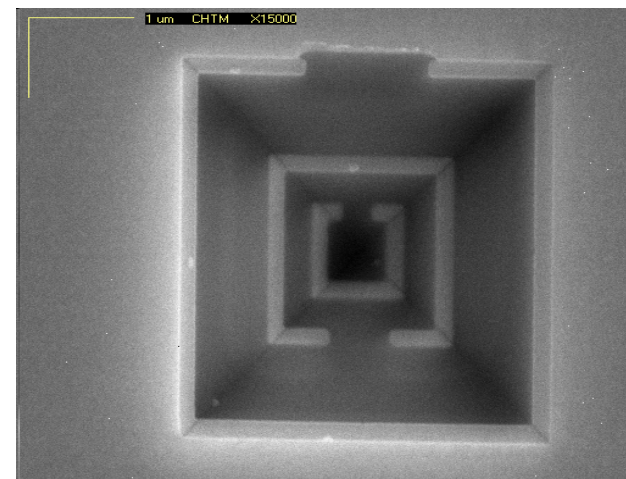
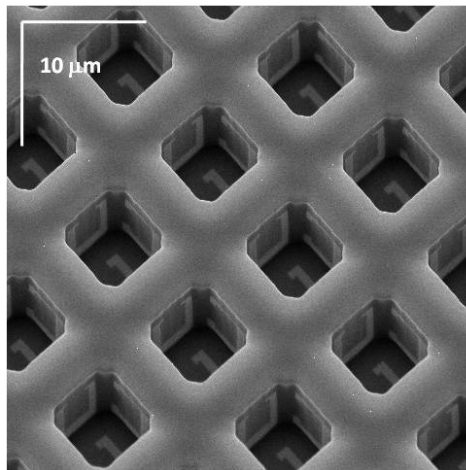
# Other Presentations from our project at META'10



**Igal Brener:** “Phase and amplitude resolved characterization of IR metamaterials and metamaterial-based modulators” → this session

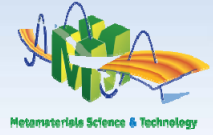


**D. Bruce Burckel:** “3-D Metamaterial fabrication using membrane projection lithography” → session 6A tomorrow



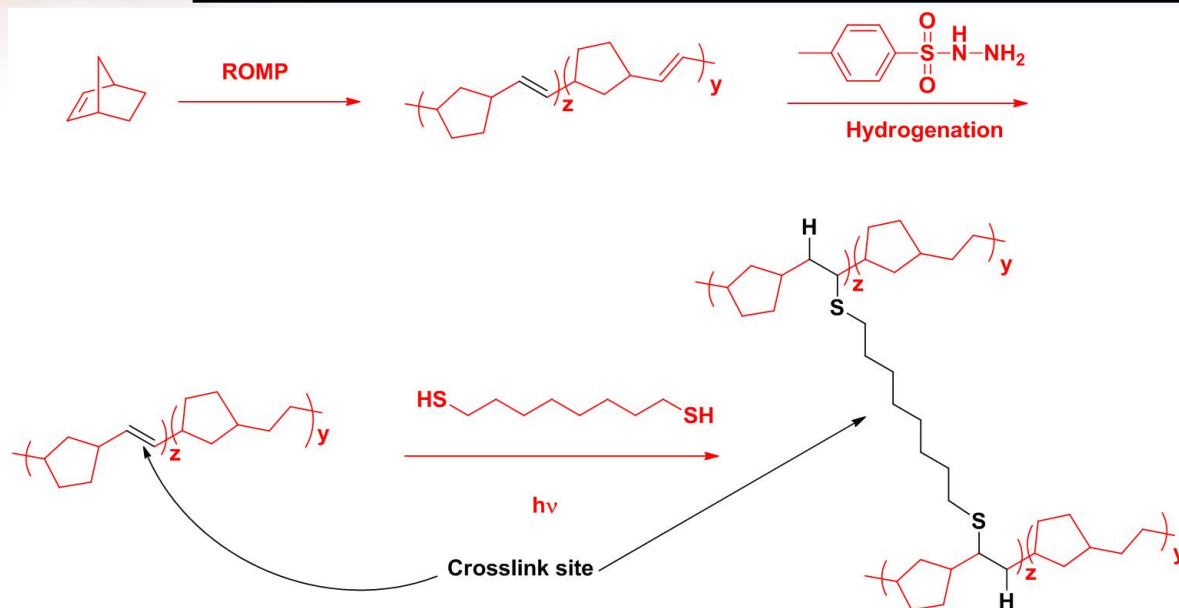


# Outline

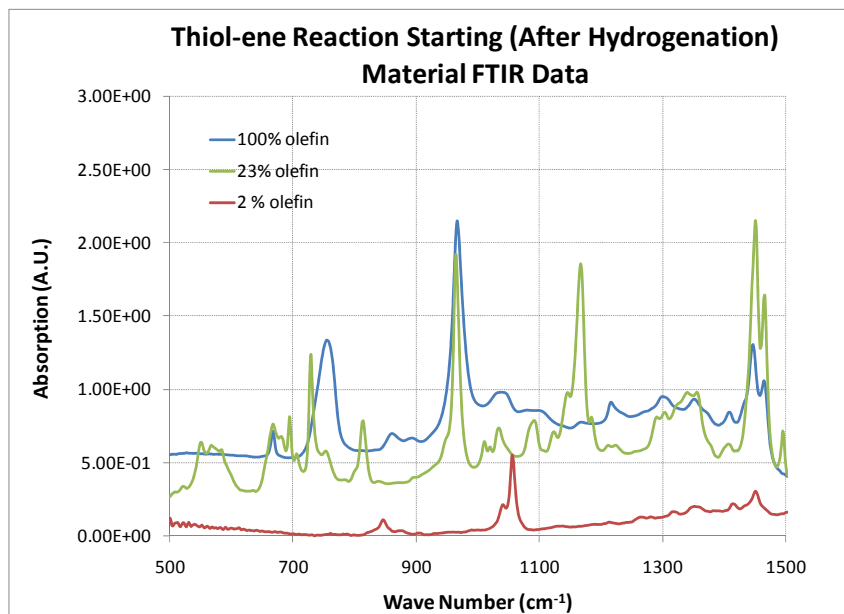


1. Sandia's Metamaterial program
  - Overview
  - Highlights: subcells/hpc
  - Highlights: low loss polymers
2. Losses of Metal-Based Metamaterials
  - stranding to reduce ohmic losses
3. Dielectric resonator based metamaterials
  - DR basics
  - DR based magnetic metamaterials
  - fundamental limitation/restrictions
  - Core/shell negative index
  - A—B sphere lattices → RF demo
  - spheres embedded in lossy lattice/negative n metamaterial

# Low IR Absorbing Photo-Patternable



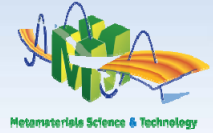
- norbornenering opening metathesis polymerization
- Controlled hydrogenation prior to crosslinking with the thiol-ene coupling reaction provides control over the amount of crosslinking and thus access desired materials properties
- final backbone resembles polyethylene



IR absorption expected to be as low as polyethylene, but:

- better solubility
- photopatternable
- cross-linked

# Finite Metallic Conductivity Complicates Numerical Modeling

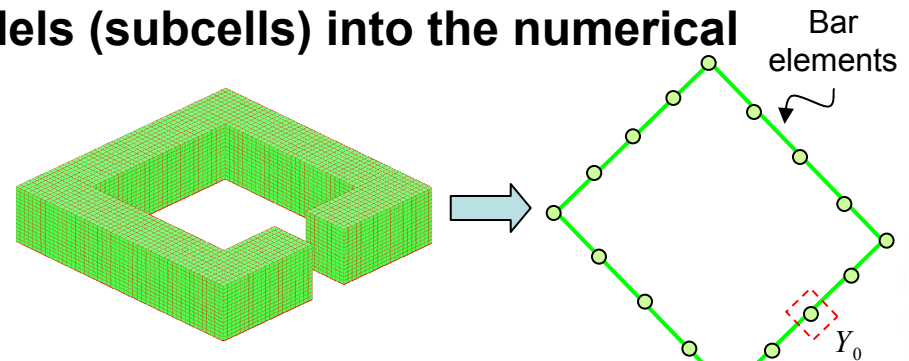


➤ **Problem:** Fine mesh required for convergence slows numerical simulations and prevents simulation of larger scale structures (e.g. Boeing prism)

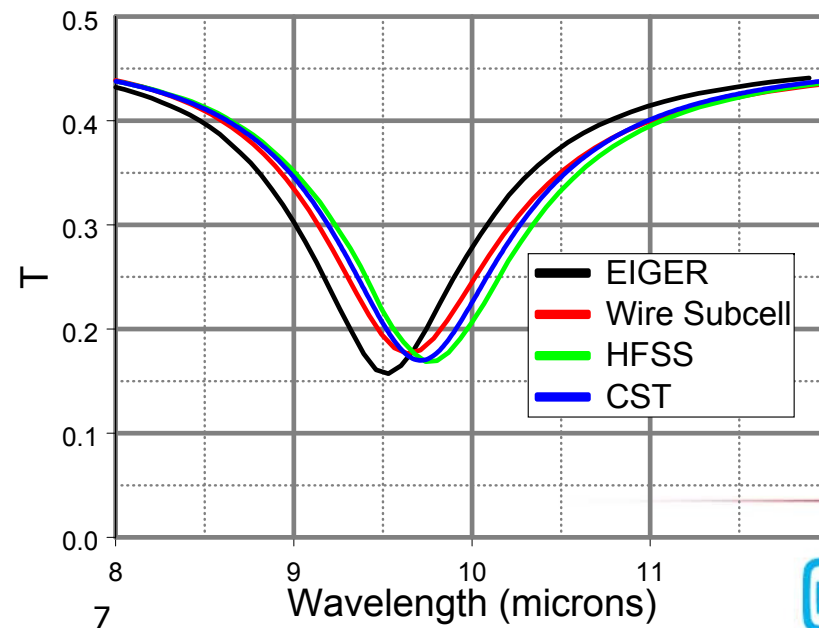
- difficult to model devices, gradients, surface effects

➤ **Solution:** Embed analytic circuit models (subcells) into the numerical simulation software

- Sandia's EIGER™ MOM code
- Dramatic (~1000X) improvement
- Viable to HPC simulation of large numbers of unit cells



SRR Design B Transmission Coefficient



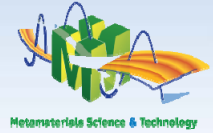
## EIGER

Explicit Mesh- Au SRR meshed as a lossy-dielectric block (surface mesh)  
3.5 hours/frequency  
29,880 unknowns & 64 processors

## EIGER Wire

Subcell Model- Au SRR modeled with wires and analytic circuit elements (impedance/length & radius of rectangle on dielectric substrate)  
8 seconds/frequency  
32 unknowns & 1 processor

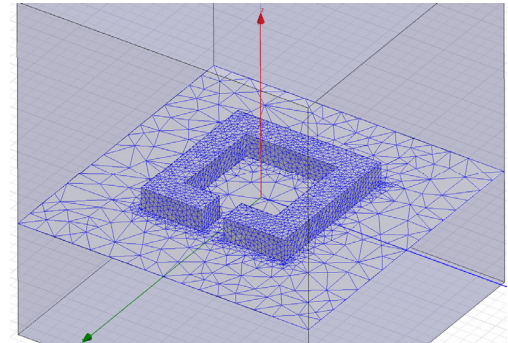
# HPC Simulation of Metamaterials



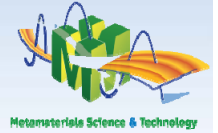
- The design of metamaterial devices typically has relied on extraction of the effective properties from simulation of *infinite periodic arrays* of identical unit cells.
- In the *infrared frequency regime* even a unit-cell analysis can lead to prohibitively large computational problems.
  - *subcell models* can be advantageous
- Using Sandia HPC resources, we perform *direct numerical simulations* of *finite metamaterials* to understand the implications of finite metamaterials, such as
  - boundary effects
  - effects due to loss in the host (introducing field gradients)
  - whole-device simulation
- We have designed *3D absorber* and *negative-index* metamaterials based on effective media theory, with HPC simulations showing favorable performance.



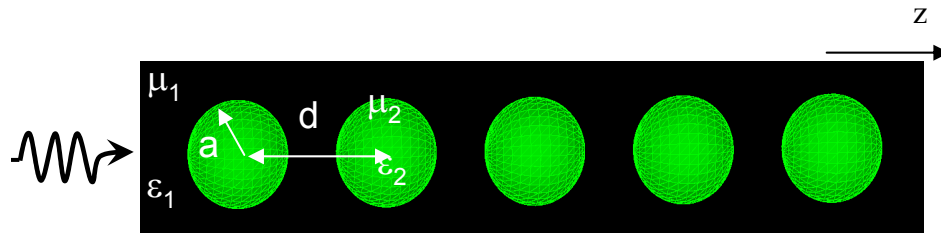
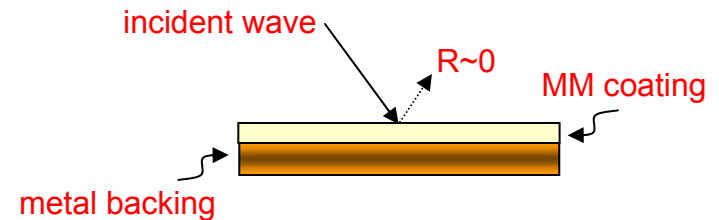
(THUNDERBIRD:  
53 Tflop, 8690  
processors)



# 3D Metamaterial Absorbers

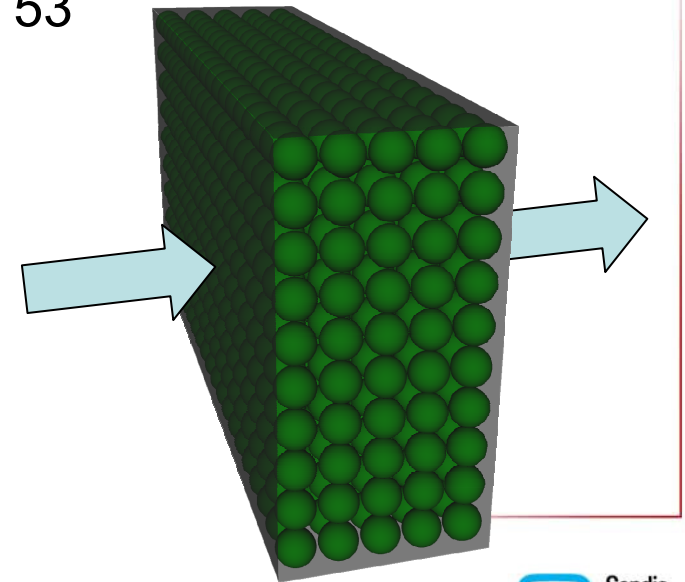


- Finite absorbing slab (5 unit cells thick) of impedance matched ( $\varepsilon = \mu$ ) metamaterial.
  - designed to hide the back interface
  - lossy dielectric spheres in a lossy medium
  - magnetic resonance of the spheres
  - matched for normal incidence at  $10\ \mu\text{m}$
- Initial design developed using effective media theory
- EIGER™ MOM Code: surface mesh scale  $\sim \lambda/100$
- Simulated on Thunderbird (8690 processors / 53 TFLOPS)
  - didn't use the whole machine for this run



$$a = 0.5\ \mu\text{m}, d = 1.5\ \mu\text{m}, \mu_{r1} = \mu_{r2} = \mu_0$$

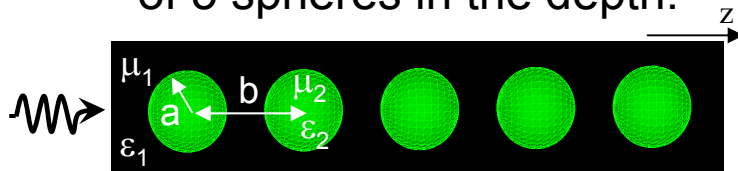
$$\varepsilon_{r1} = 2.19 + i0.68, \varepsilon_{r2} = 91 + i1.82$$





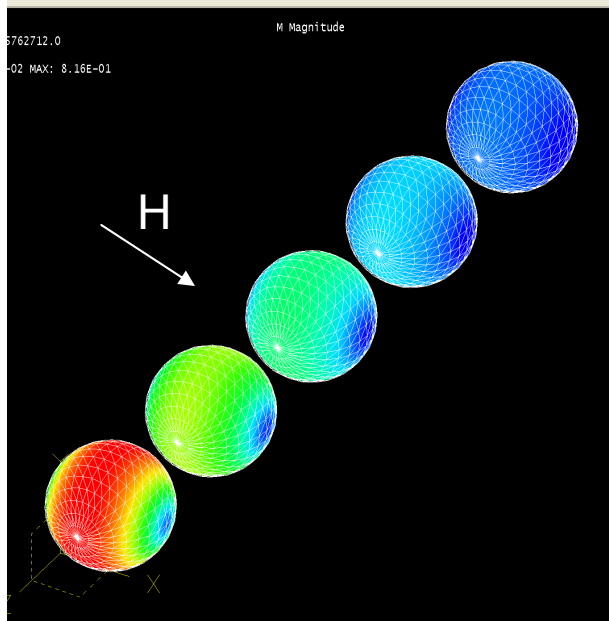
# Absorber Design #1

**Design:** An absorbing layer composed of 5 spheres in the depth.

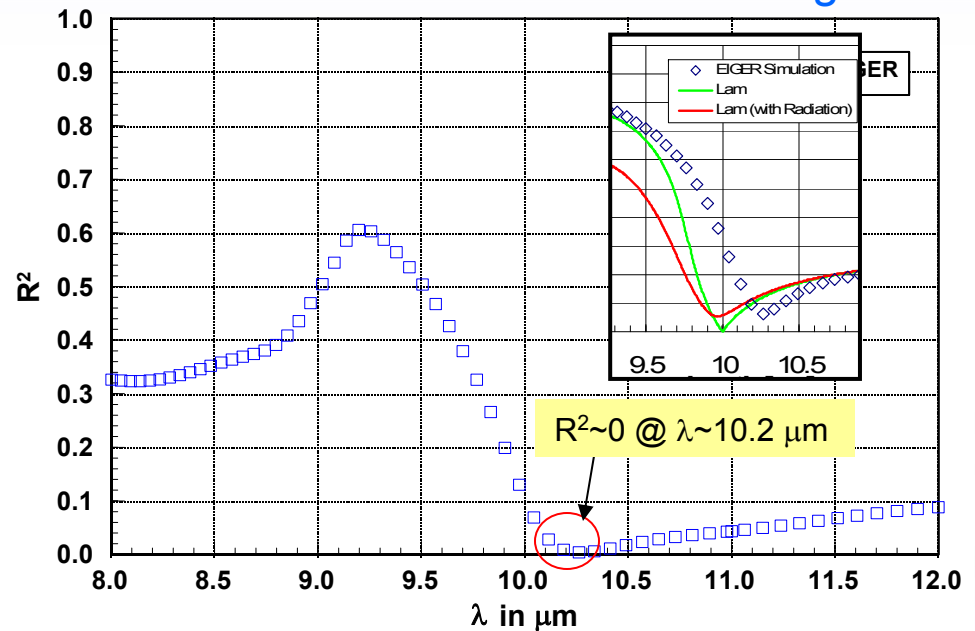


$$a = 0.5 \mu m, b = 1.5 \mu m, \mu_1 = \mu_2 = \mu_0$$

$$\epsilon_{r1} = 2.19 + i0.68, \epsilon_{r2} = 91 + i1.82$$



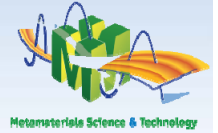
## Reflected Power versus Wavelength



Impedance matched reflectance minimum is observed at the design wavelength

- Have also simulated
  - 5-layer SRR absorber
  - 5-layer negative index slab
- Working towards device level modeling
  - Boeing prism??

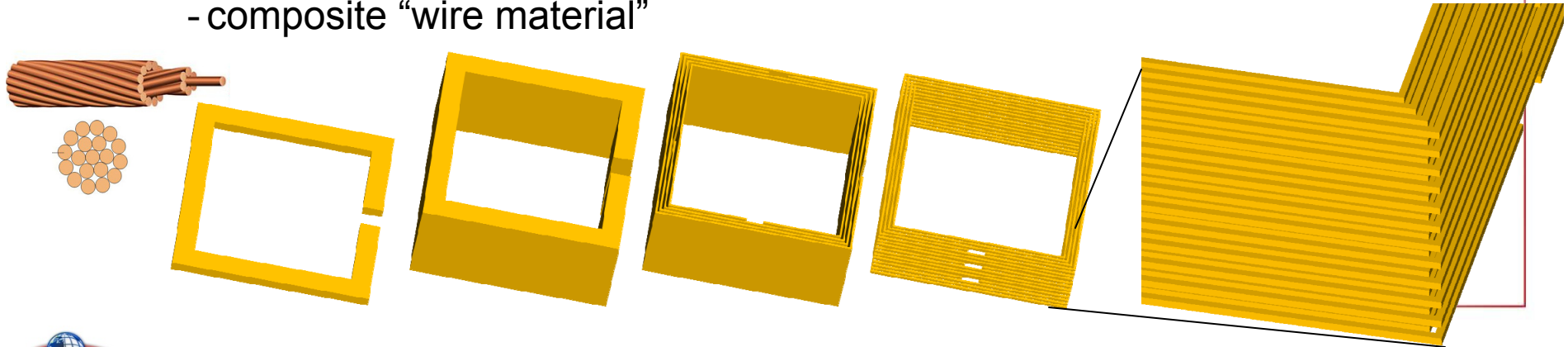
# Metal-Based Metamaterials



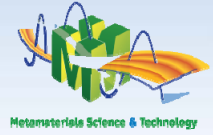
- Metal metamaterials are the easiest to fab → we have a good 3D route
- Electronic scattering → Ohmic losses → Metamaterial loss
- It is essential understand the performance limits for metal-based metamaterials

## Study of fundamental loss limits vs. $\epsilon$ and $\mu$ is ongoing:

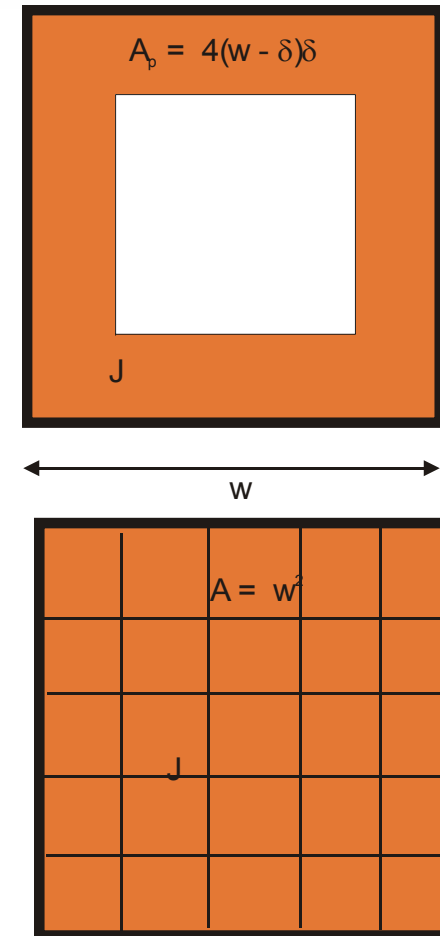
- Graded approach:
  - “back of the envelope” →  $I^2R$
  - Cummer → “Q-Based Design” →  $I^2R$  & parameterized  $\mu$
  - Tretyakov, Boardman, etc → “Poynting Theorem in Dispersive Media” & parameterized  $\mu$  &  $\epsilon$
  - Design and model an optimal structure
- We believe that lowest loss will be achieved through maximum “stranding” to distribute currents, lower R, and increase Q
  - composite “wire material”



# Loss Conclusions

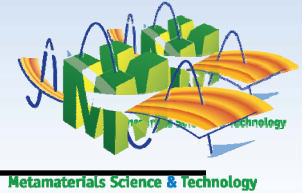


- Metal Design Bulk Media Permeability Loss Tangent Near Unity
  - Stranding in mid IR not very effective at reducing this level (unlike in THz or lower frequencies) (1.5 times increase in area illustrated on right)
  - Downshifting of SRR resonance can be accomplished either with dielectric gap loading or with double ring topology
- Dielectric Resonators lead to bulk permeability loss tangents that are more than an order of magnitude less (for a cubic lattice)



# Compromises Between Cell Size and Low-Loss Metal Design

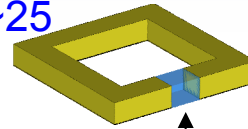
## Magnetic Permeability



$$\tan \delta_{eff} = \frac{\mu_{eff}''}{\mu_{eff}'} \sim \frac{24}{Q} \approx 0.5 - 1 \quad (\mu_{eff}' = -1)$$

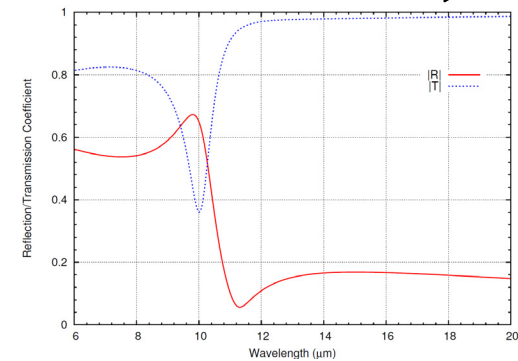
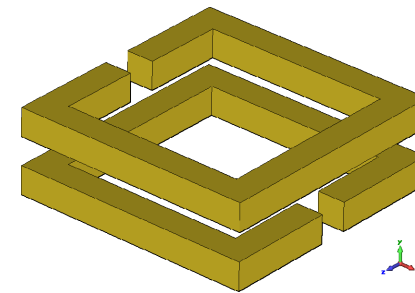
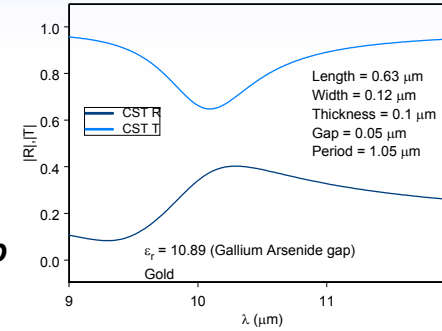
Clausius Mossatti  $\tan \delta_{eff}$

$Q_{loss} \sim 25$



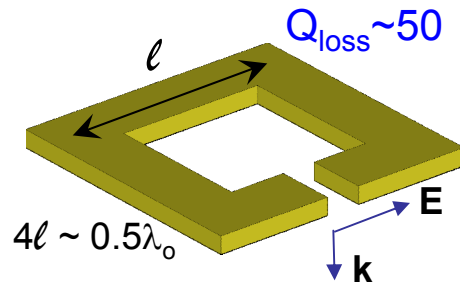
$$4\ell \sim 0.25\lambda_0$$

GaAs loaded gap



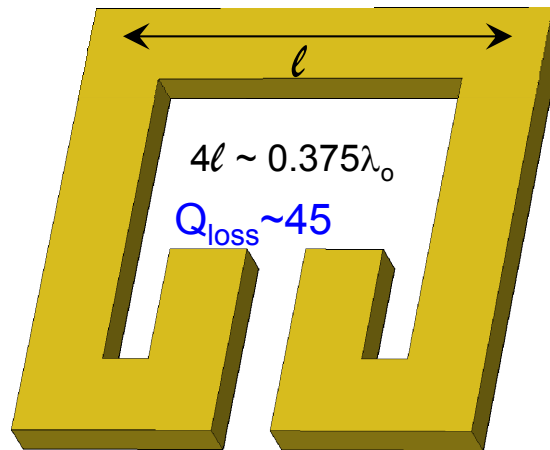
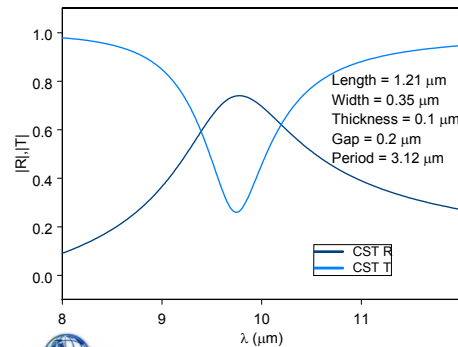
$$4\ell \sim 0.3\lambda_0$$

$Q_{loss} \sim 30$

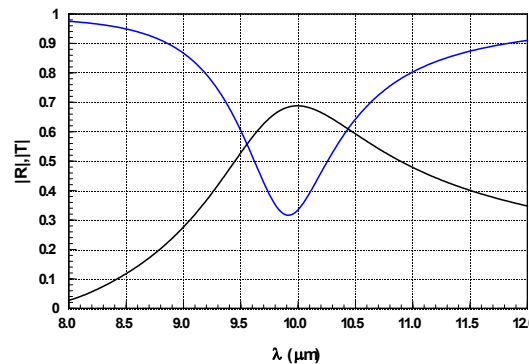


$$4\ell \sim 0.5\lambda_0$$

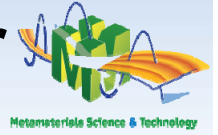
Air SRR



Bent-Arm SRR



# Low Loss Strategy: Dielectric Resonator Metamaterials



***Electromagnetic scattering by arrays of high- $\epsilon$  resonators can lead to low loss electric and magnetic metamaterials.***

## **Dielectric Spheres $\rightarrow$ Mie scattering**

- electric & magnetic dipole resonances
- occur at different frequencies

## **Array of resonators in a host matrix:**

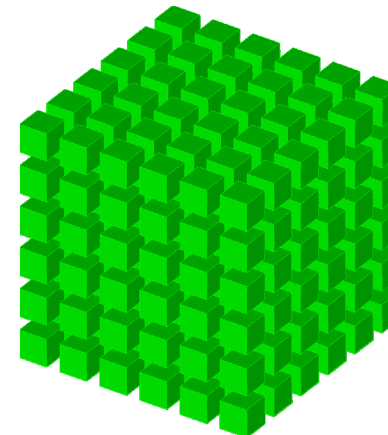
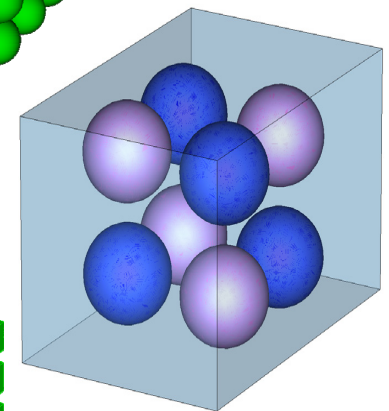
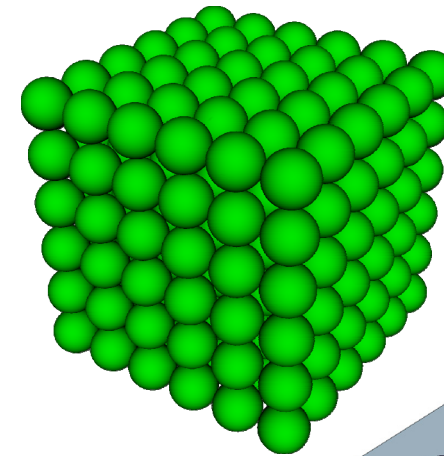
- effective  $\epsilon$  and  $\mu$  values
- Claussius-Mossotti equation or beyond

## **Overall loss depends on loss tangents of resonators and host**

- can be significantly lower than metal based metamaterials.

## **Other resonant scattering structures can be employed**

- cubes
- wires
- anisotropic structures
- readily extendible to IR metamaterials



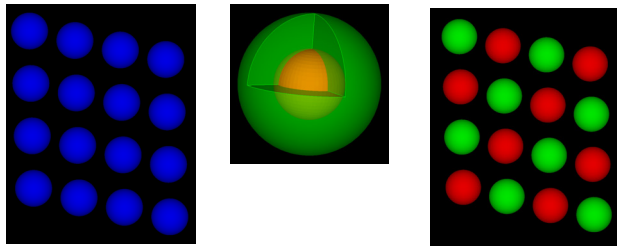
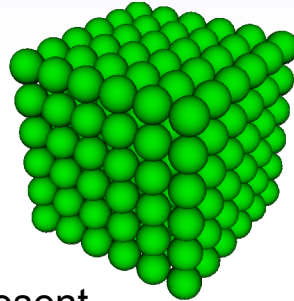


# Effective Media Models

## *MM Design and Guiding Retrieval*

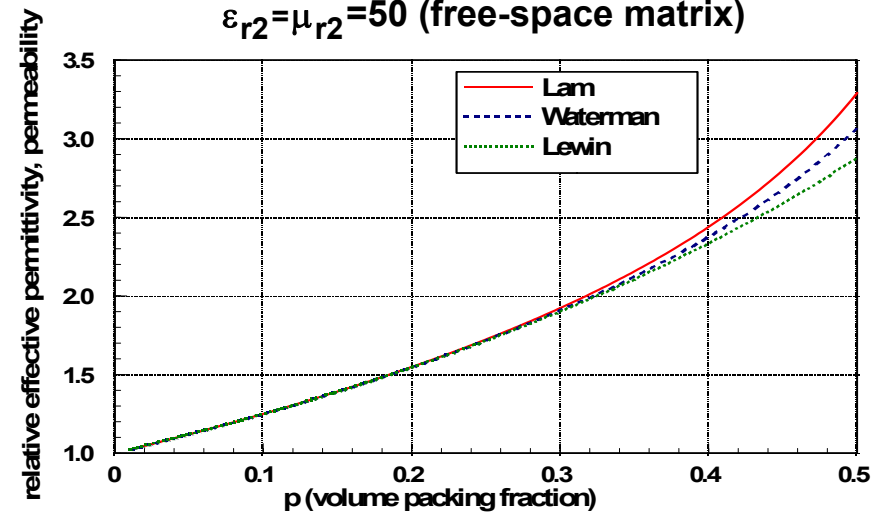


- Quasistatic result
  - Lam
  - Duality
  - Clausius-Mosatti
  - Waterman
  - Holloway & Kuester
- Types of structures at present
  - Spheres
  - Core-shell structures
  - Two-species spheres



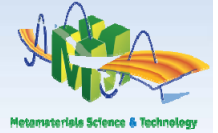
- Dynamic host corrections
  - Low-frequency expansion host (Draine, Tretyakov, Shivola)
  - Radiation (Layer, Sipe)
  - Effective media cutoff (Lerat, Koschny)

**Spherical Particle Array ( $ka=0.1$ )**  
 $\epsilon_{r2}=\mu_{r2}=50$  (free-space matrix)

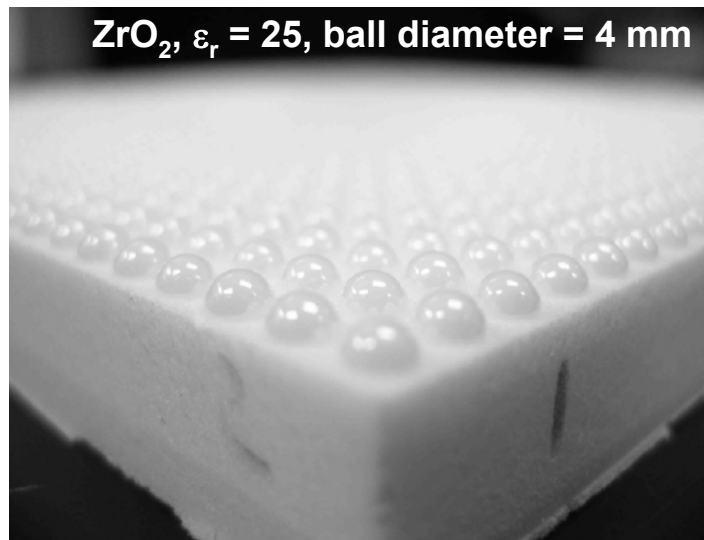


J. Lam (J. Appl. Phys. 60 (12), 1986)  
P. Waterman et. al (J. Appl. Phys. 59, 1986)  
L. Lewin (Proc. Inst. Elec. Eng. 94, 1947)  
C. Holloway (IEEE Trans. Antennas Propag. 48, 2000)

# RF demonstration of a magnetic metamaterial

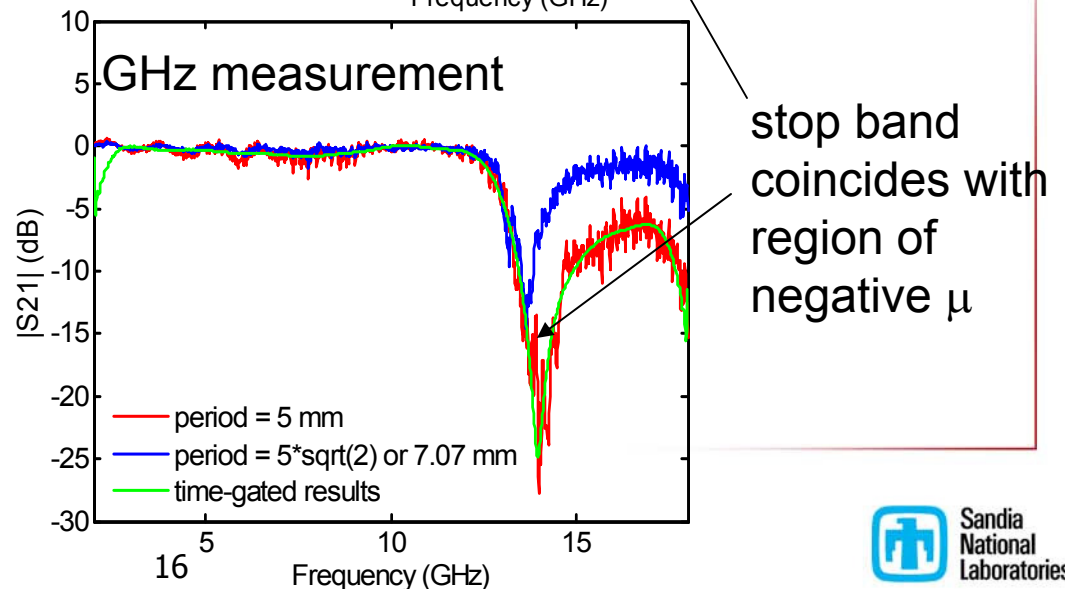
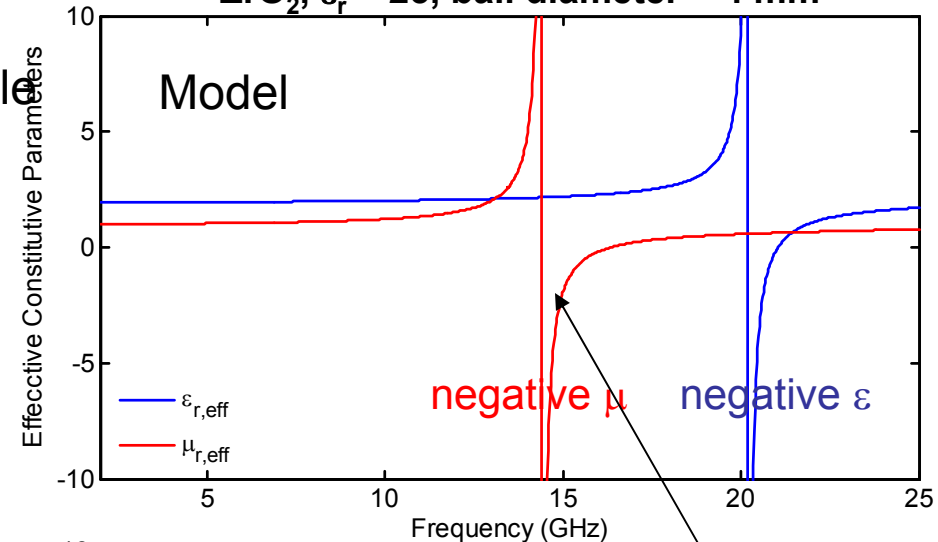


- **RF is a good test bed for metamaterial development**
  - high  $\epsilon$  materials readily available
  - macroscopic dimensions
  - easy test
- **Path to IR**
  - lithography → cubes



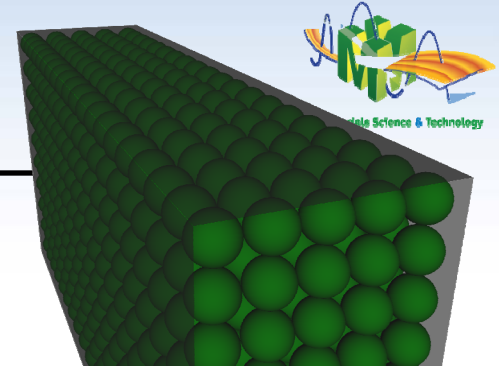
Example: Negative  $\mu$  metamaterial.

$\text{ZrO}_2$ ,  $\epsilon_r = 25$ , ball diameter = 4 mm



# PbTe Sphere Simulations: Summary of Results

Host Material is Air for Permeability  
Only



Dielectric Sphere Design	$\lambda$ in $\mu\text{m}$	$\text{Real}(\mu_{r,\text{eff}})$	$\text{Imag}(\mu_{r,\text{eff}})$	$ \tan \delta_m $
$a=0.89 \mu\text{m}$ , $b=2.28 \mu\text{m}$ , $\epsilon_r=(32.04, 0.0566)$ $\tan \delta_{\text{PbTe}}=0.0016$	9.89	-1.01 (no rad)	0.0306 (no rad)	0.0306 (no rad)
$a=0.89 \mu\text{m}$ , $b=2.28 \mu\text{m}$ , $\epsilon_r=(32.04, 0.0001)$ $\tan \delta_{\text{PbTe}}=3.12\text{e-}6$	9.89	-1.01 (no rad)	$5.40\text{e-}5$ (no rad)	$5.40\text{e-}5$ (no rad)

$$k'a = \pi(1 + \Delta)$$

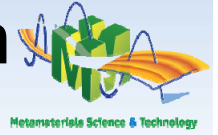
$$\mu_{\text{eff}} / \mu_0 \sim -2 + (2\Delta + i \tan \delta) \pi^2 / p$$

$$p = 4\pi a^3 / (3b^3)$$

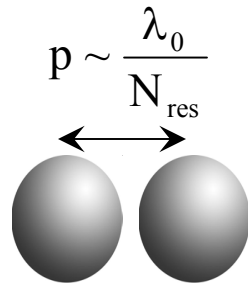
For negative unity real part

$$-\tan \delta_{\text{eff}} \sim (\pi^2 / p) \tan \delta$$

# Effective Parameters Limitations with Dielectric Resonators



- Largest identified  $\epsilon$  in thermal IR is not as high as is desired
  - extending effective medium theory to account for finite size effects
- Minimum resonator size & pitch  $\sim \lambda_0/N_{\text{res}}$

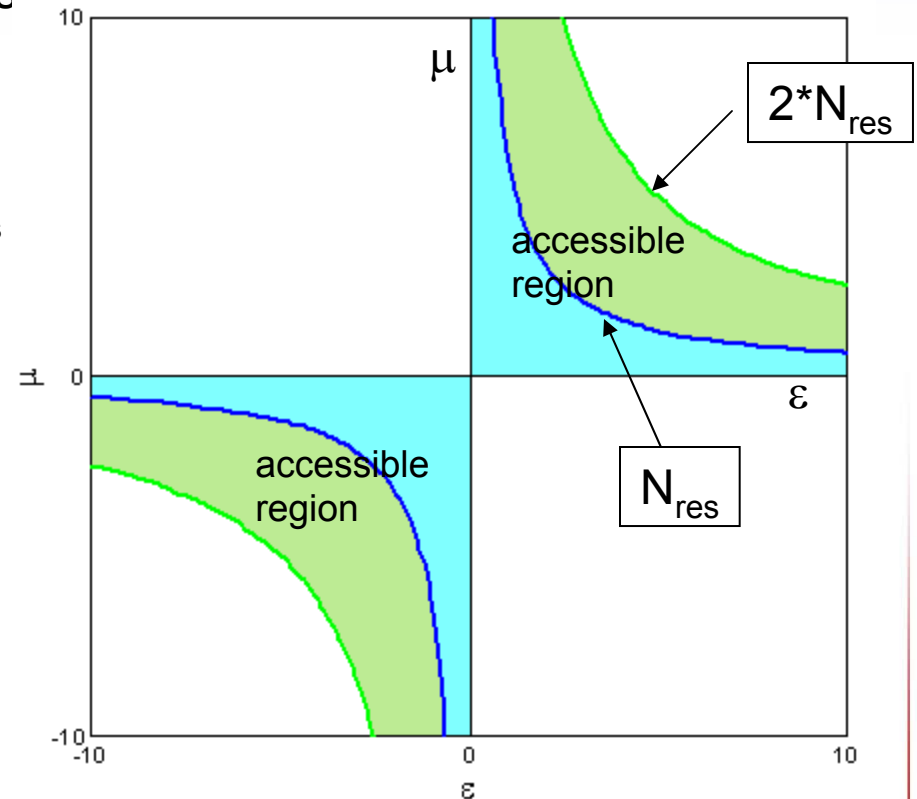


- Effective medium wavelength must be greater than twice the pitch

$$\lambda_{\text{eff}} = \frac{\lambda_0}{N_{\text{eff}}} > 2 \cdot p \approx 2 \cdot \frac{\lambda_0}{N_{\text{res}}}$$

- Accessible region of  $\mu$ - $\epsilon$  space correspond to:

$$N_{\text{eff}} \leq \frac{N_{\text{res}}}{2}$$



- Larger values of  $N_{\text{res}}$  give access to more  $\mu$ - $\epsilon$  space
- ENZ, MNZ accessible

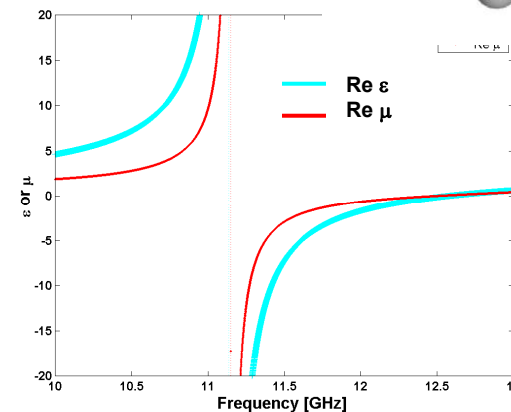
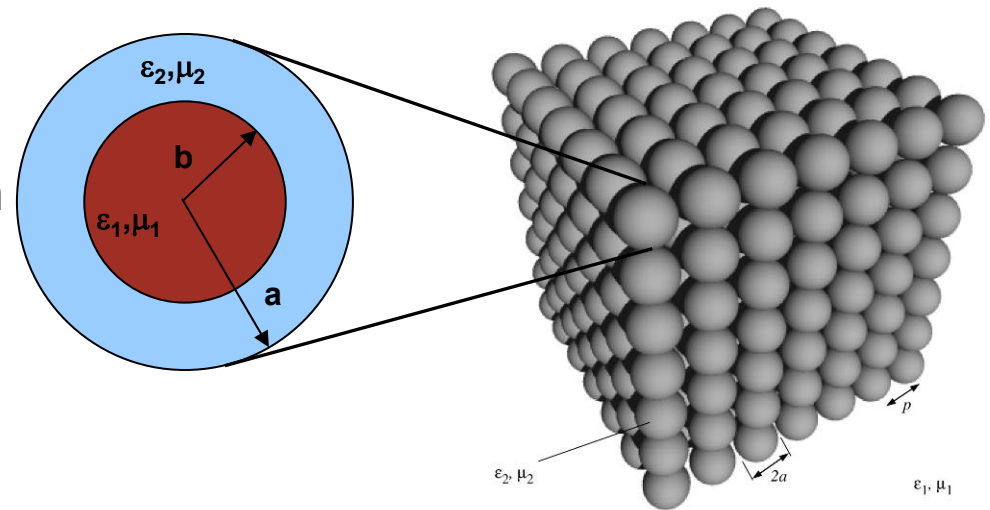
# Achieving negative index behavior with dielectric resonators: core/shell metamaterials



**Combining materials and structures allows independent tuning of  $\epsilon$  and  $\mu$ .**

- Dielectric core/shell particles.
- By adjusting the radii and materials in a core/shell configuration, the electric and magnetic resonances can be brought into coincidence.
- Isotropic, low loss material
- Demonstrates ability to have a negative index without metals.

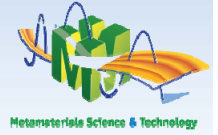
Drawback: particles are difficult to fabricate  
→ experimental verification difficult



$a = 4.66 \text{ mm}; b = 2.25 \text{ mm}; p = 2.013a$   
 $\epsilon_2 = 9.5; \epsilon_3 = 100; \tan \delta_2 = 2 \times 10^{-4}; \tan \delta_3 = 10^{-3}$   
calculation by Ed Kuester, U. of Colo.



# Alternate approach: two-species metamaterials



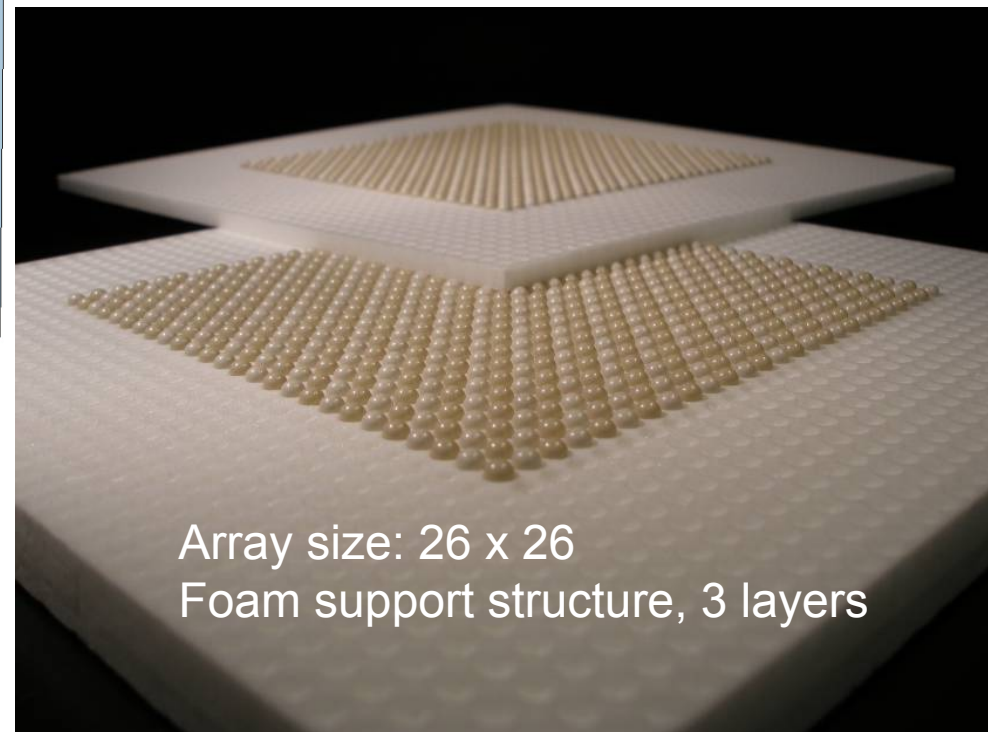
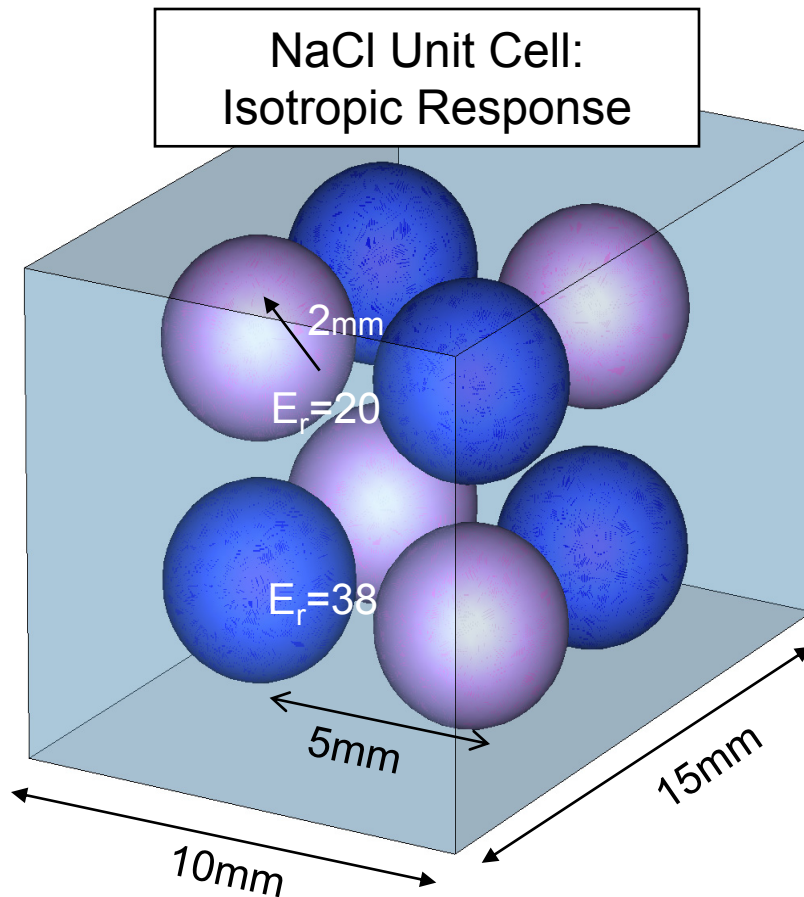
- Overlap the magnetic dipole resonance of one species with the electric dipole resonance of the other

Blue:  $(\text{Zr}, \text{Sn})\text{TiO}_4$

- $\epsilon_r=38$
- electric resonance

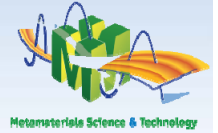
Pink:  $(\text{Mg}, \text{Ca})\text{TiO}_3$

- $\epsilon_r=20$
- magnetic resonance

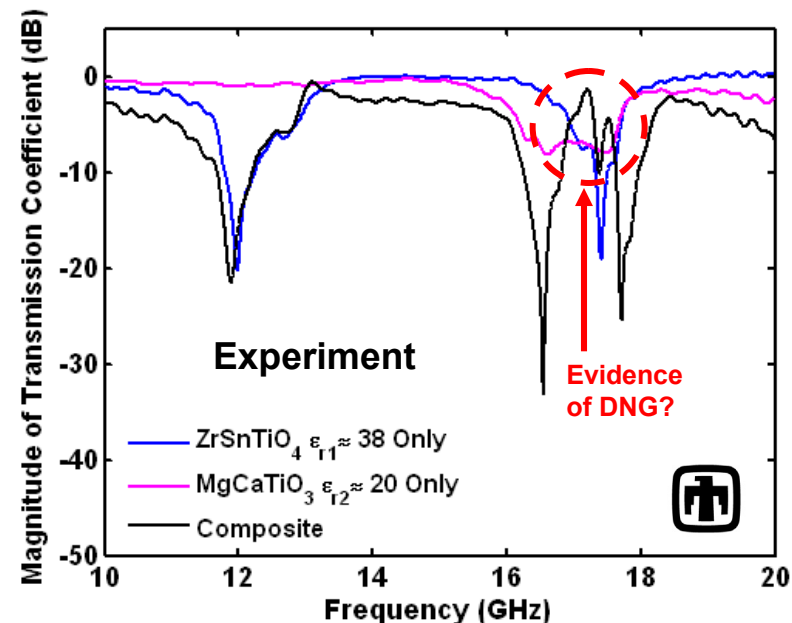
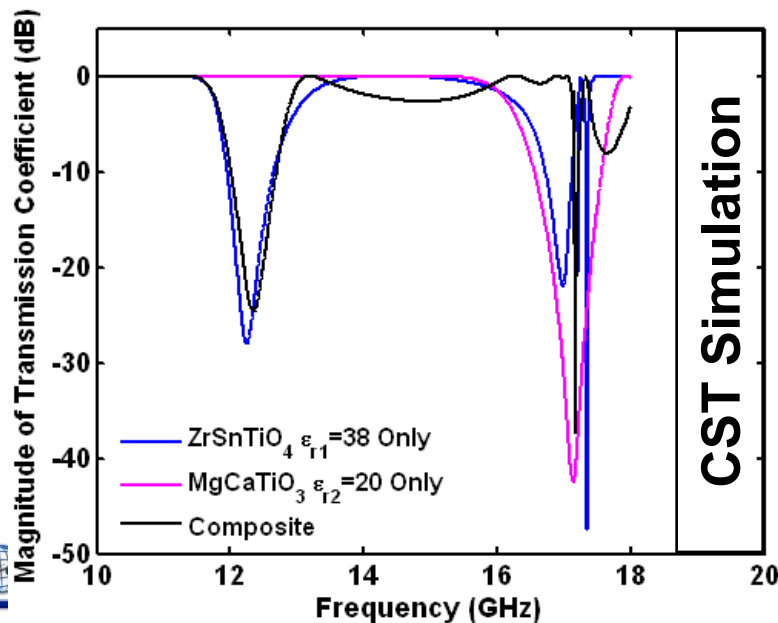
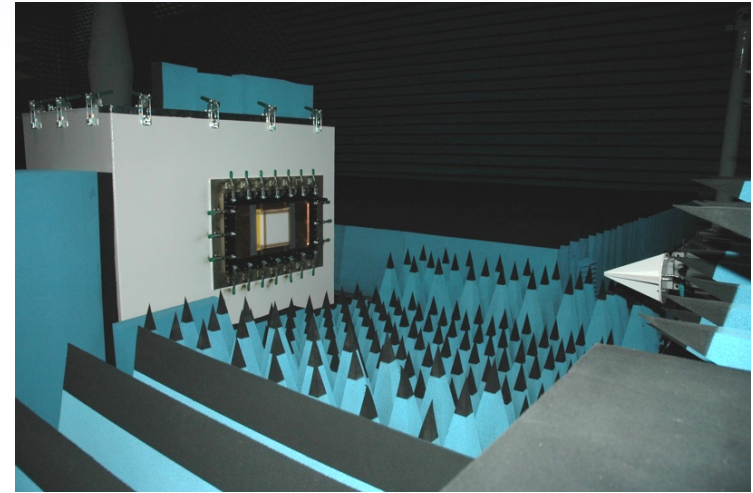


Array size: 26 x 26  
Foam support structure, 3 layers

# RF Characterization of DNG Array

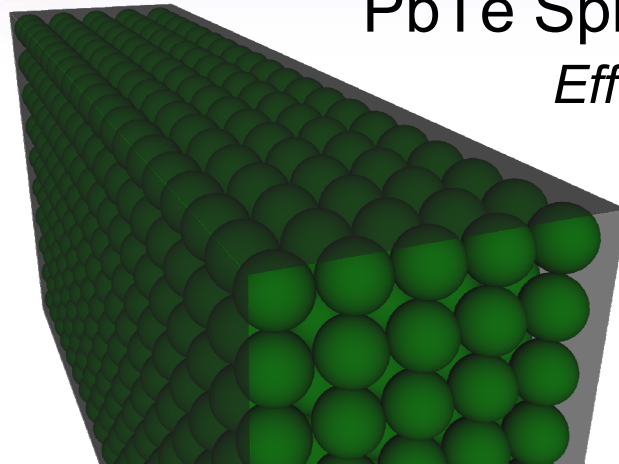


- Transmission bands appear where band-stops of the two spheres overlap → DNG?
- Observed behavior is more complex than expected
  - Drawback: unit cell size doubles with two-species approach --- problems when effective medium  $\lambda$  becomes small
- Analysis of DNG behavior is continuing
- Core/shell spheres & DNG prism



# Third approach to negative index: high-Q resonators in $\epsilon < 0$ matrix

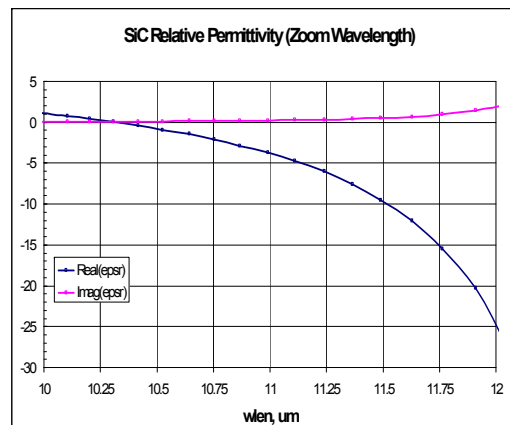
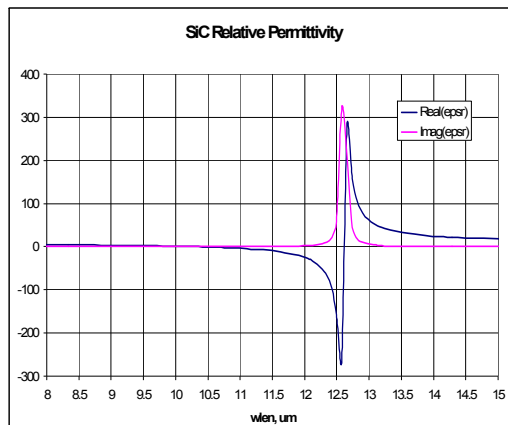
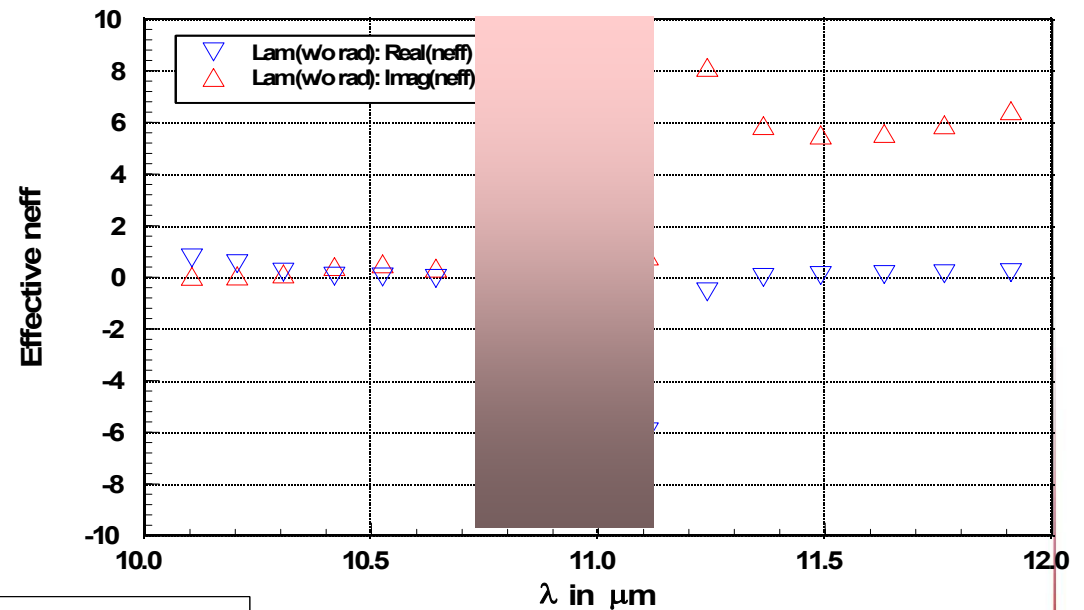
## PbTe Spheres in SiC Host Layer *Effective Media Design*



$$a = 0.997 \mu\text{m}, b = 3.467 \mu\text{m}, \mu_1 = \mu_2 = \mu_0$$

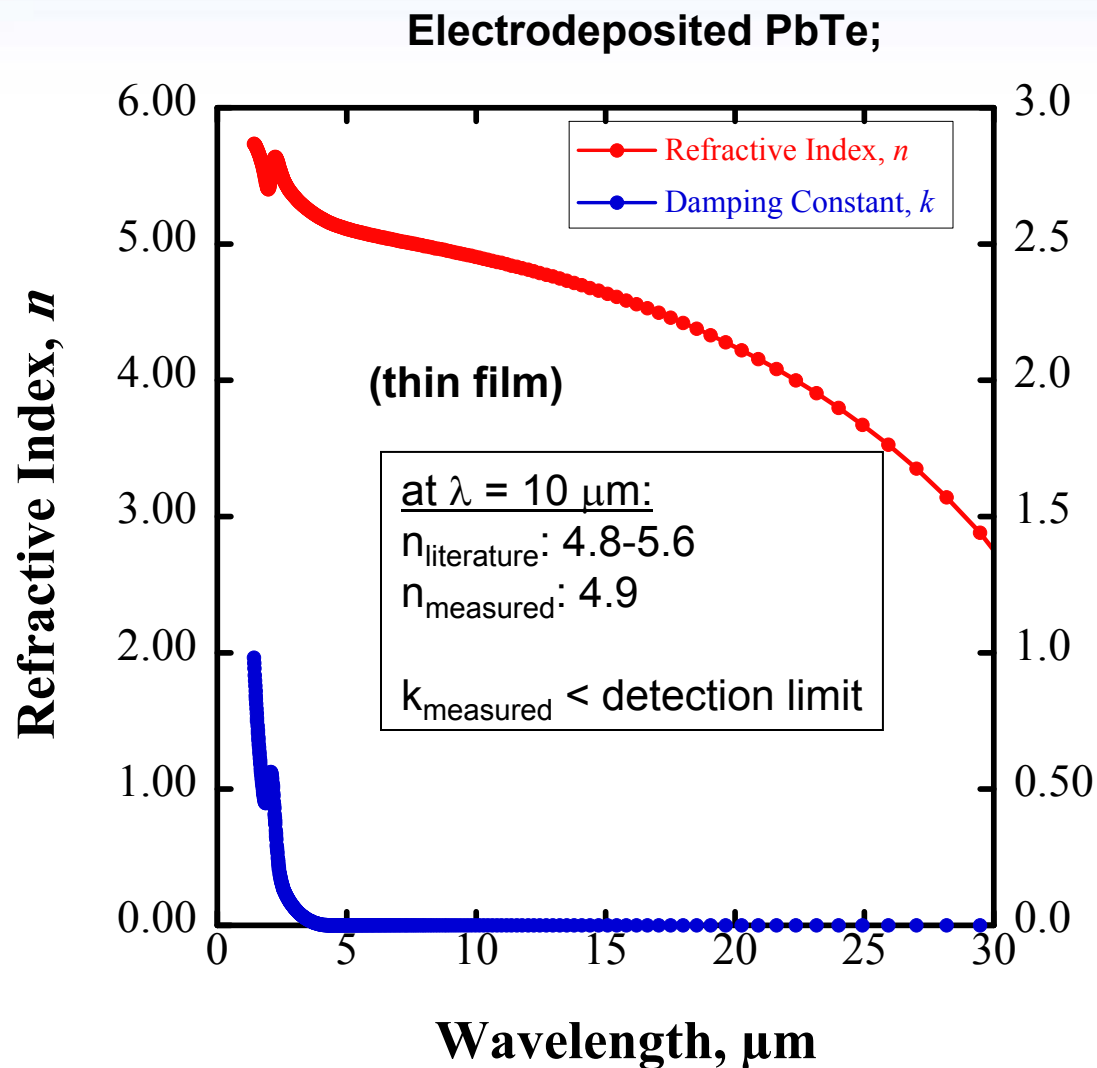
$$\epsilon_{r1} = \epsilon_{r1}(f), \epsilon_{r2} = 30.5 + i0.0734$$

- Palik values for PbTe
- SiC dispersion



wlen, um	real(neff)	imag(neff)	FOM	dB/wlen
10.5246	1.91E-02	0.522051	0.04	28.49095
10.6421	-4.26E-02	0.355347	-0.12	19.39307
10.7528	-0.69219	9.55E-02	-7.25	5.213459
10.8659	-1.47574	0.130098	-11.34	7.100115
10.9911	-2.79201	0.239538	-11.66	13.07281
11.1093	-5.98391	0.833036	-7.18	45.46297

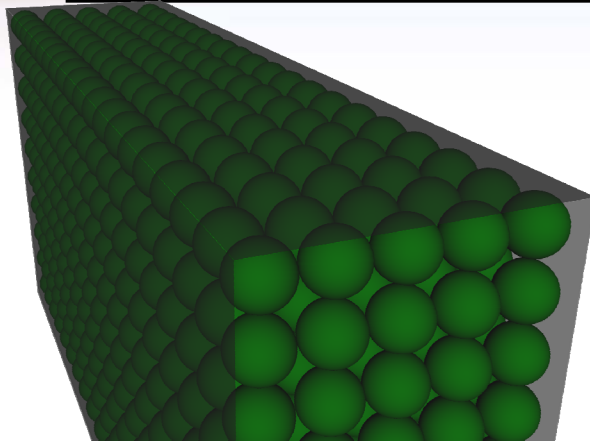
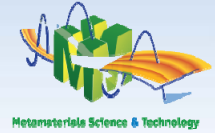
# Measured optical constants of PbTe : IR VASE



Measured optical loss is significantly lower than Palik values

# PbTe Spheres in SiC Host Layer

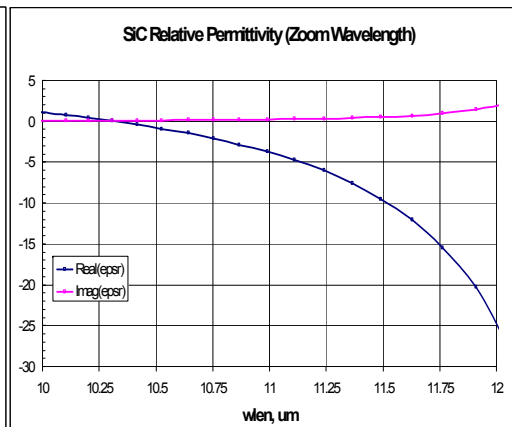
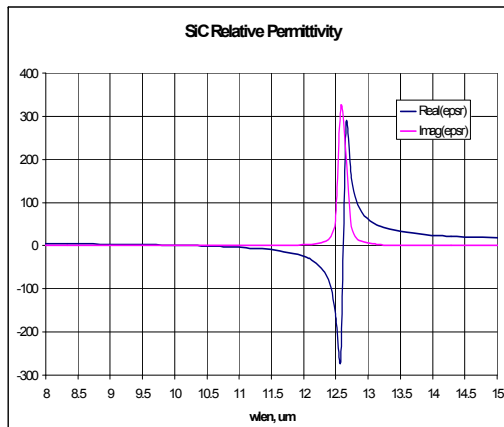
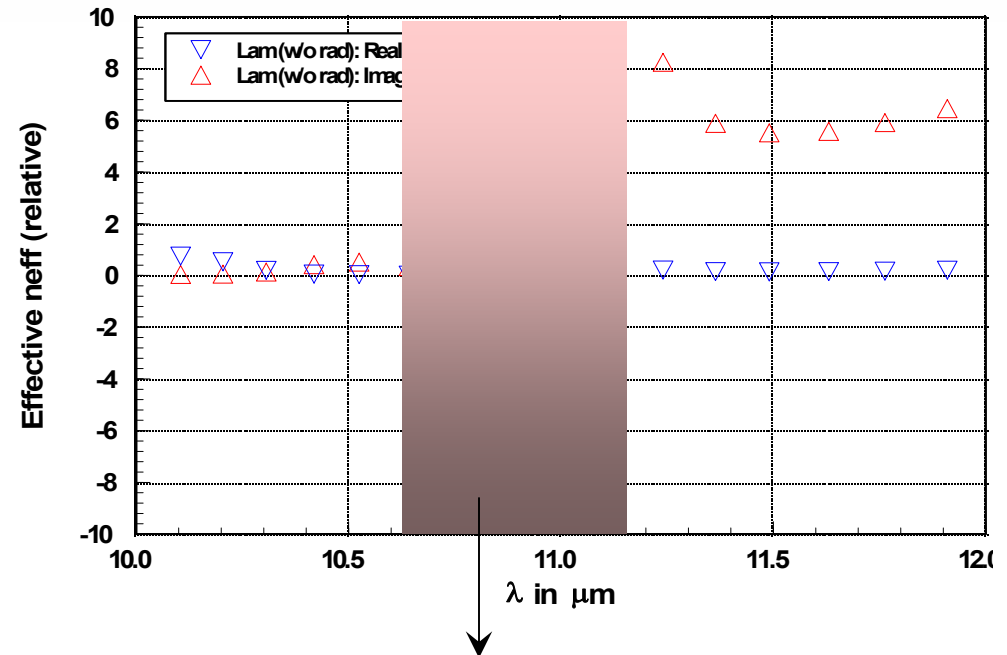
## Effective Media Design



$$a = 0.997 \mu\text{m}, b = 3.467 \mu\text{m}, \mu_1 = \mu_2 = \mu_0$$

$$\epsilon_{r1} = \epsilon_{r1}(f), \epsilon_{r2} = 30.5 + i0.0001$$

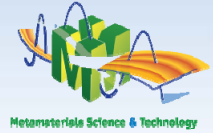
- Lower  $\tan\delta$  for PbTe
- SiC dispersion



<u>wlen, um</u>	<u>real(neff)</u>	<u>imag(neff)</u>	<u>FOM</u>	<u>dB/wlen</u>
10.6421	1.65E-02	0.345887	0.05	18.87681
10.7528	-0.69362	2.65E-02	-26.19	1.445161
10.8659	-1.47974	4.81E-02	-30.75	2.625945
10.9911	-2.80363	8.20E-02	-34.21	4.473151
11.1093	-6.09487	0.166582	-36.59	9.09124



# Summary



- Ohmic losses limit transparency of metal based metamaterials in the thermal IR
- Dielectric resonator based metamaterials are capable of lower loss, but face challenges
  - very high  $\epsilon$  resonator materials not available in thermal IR
  - resonator size & spacing must remain in effective medium limit
  - strategies to tune both  $\epsilon$  and  $\mu$  can lead to increased unit cell size
  - residual losses in resonator materials can limit achievable effective  $\tan\delta$ .