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Localized Heating Near a Rigid Spherical Inclusion in a Viscoelastic Binder Material Under Compressional Plane Wave Excitation

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Localized Heating due to Stress Concentrations Induced in a Lossy Elastic Medium via the Scattering of Compressional Waves by a Rigid Spherical Inclusion

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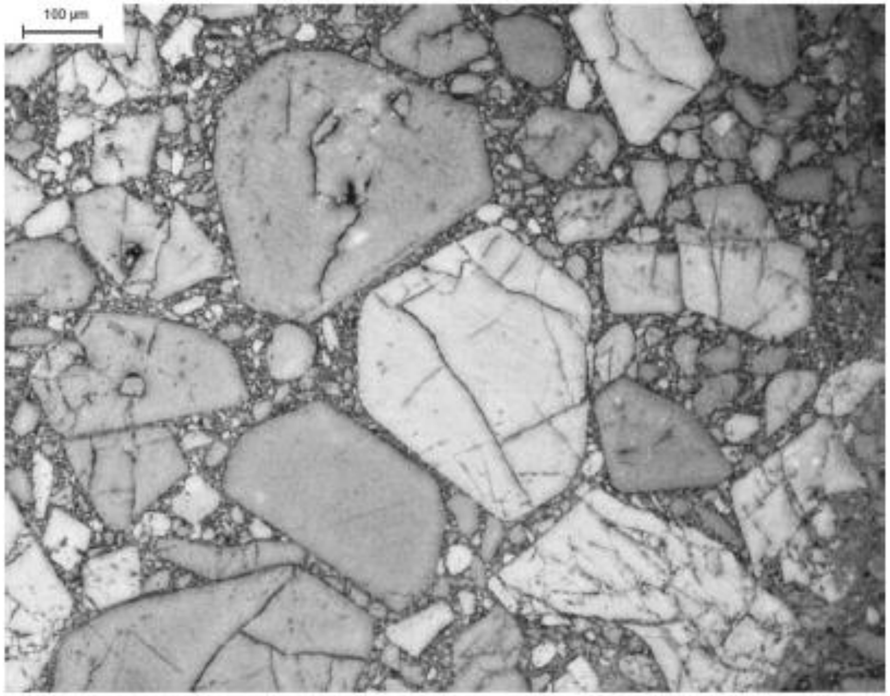
Energetic materials in a binder

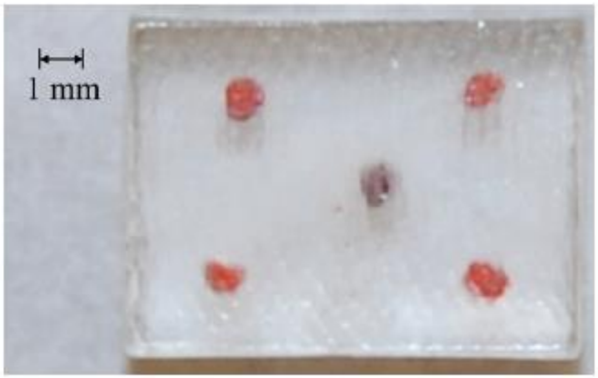
- Common use of energetic crystals involves embedding them in a binder
- Behaviors of interest include mechanical interactions between crystals, mechanical behavior of the binder and crystals separately, and interactions between the binder and crystals.
- Loading conditions include impact and periodic excitation
- Periodic excitation involves high strain-rate behaviors, even if overall strain rate is low
- Complex structure makes coupled mechanisms difficult to isolate



Micrograph of PBX 9501 (HMX in estane based binder)
Berghout, et. al., 2002, Combustion of damaged PBX explosive

Experimental Motivation

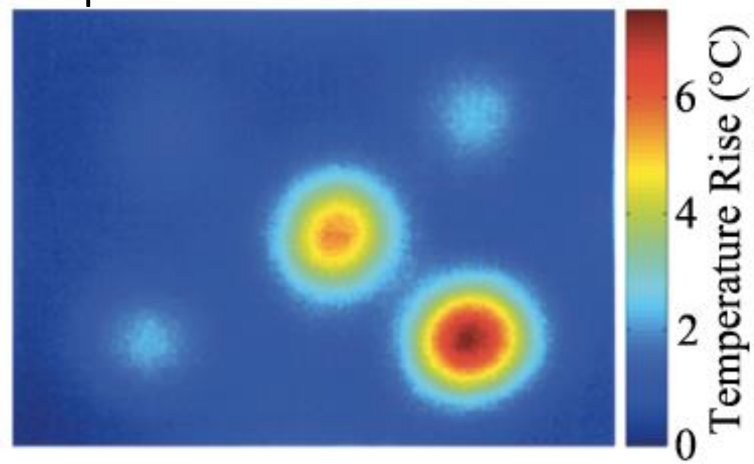
750-800 µm AP crystals to undergo excitation



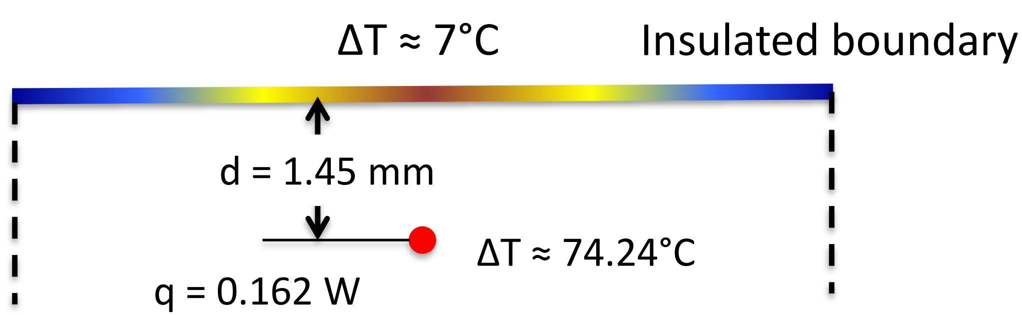
Single-crystal sample under ultrasonic excitation

(image adapted from Miller et al., J. Appl. Phys., 2016)

Surface temperature rise of 750-800 µm AP particles after 2 s excitation

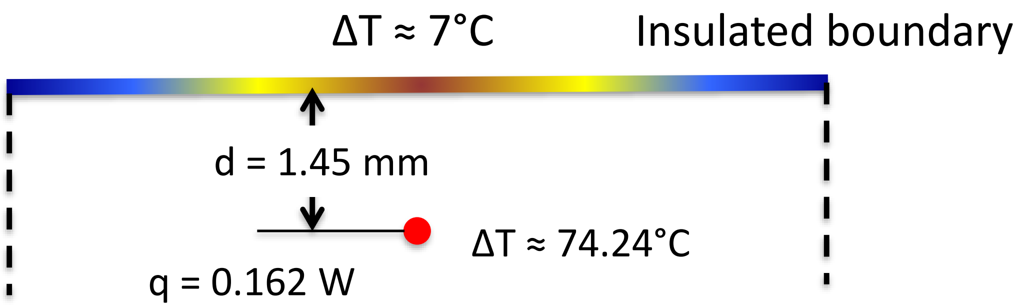


Mares, et. al., *Journal of Applied Physics* 116, 204902 (2014); doi: 10.1063/1.4902848



Point heat source in semi-infinite medium

Experimental Crystal Heating Rates



Point heat source in semi-infinite medium

- Analytical approximation using semi-infinite medium solution for heat source magnitude *q* and depth *d* (varies due to morphology)
- Particle surface temperature is found by applying the same solution with given q at the particle radius
- 37°C/s for 750-950 µm HMX in Sylgard® at 215 kHz
- 125°C/s for 400-500 µm AP in Sylgard® at 215 kHz

Mares, et. al., *Journal of Applied Physics* 116, 204902 (2014); doi: 10.1063/1.4902848

Ideal problem setup

Assumptions:

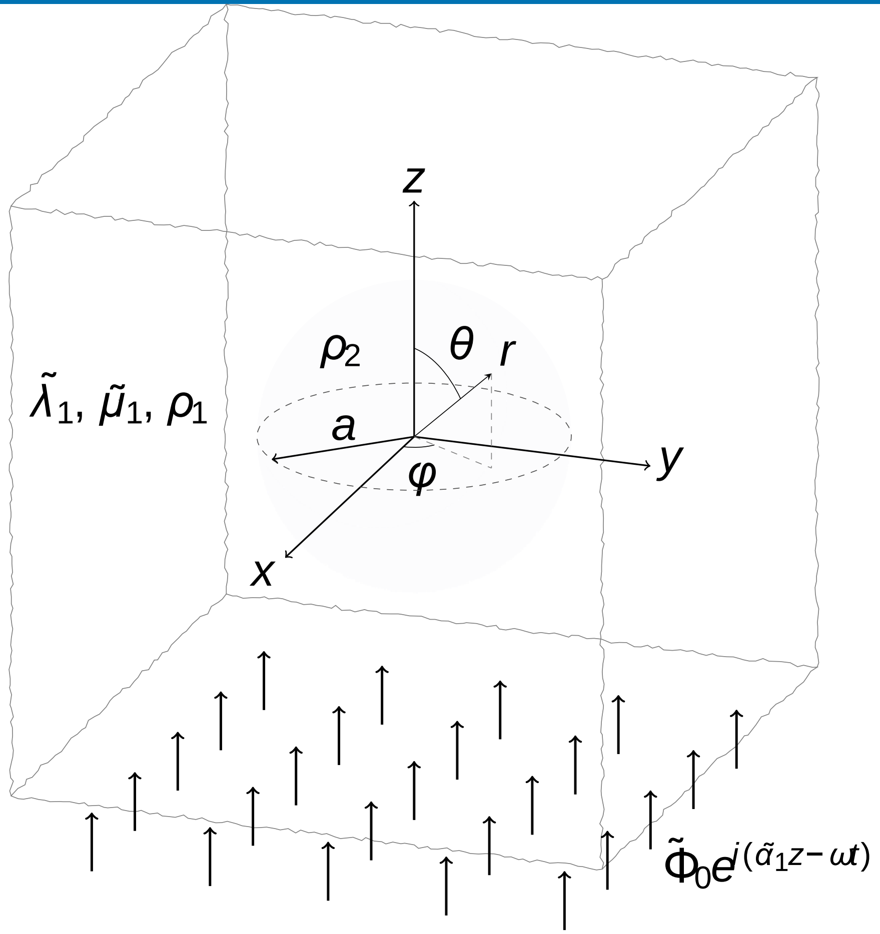
- Rigid spherical particle (no intrinsic heating)
- Linear viscoelastic binder
- Planar incident wave
- Perfect bonding between binder and particle (no particle/binder friction)
- Thermal stresses negligible
- Temperature-independent parameters

Boundary conditions:

- Displacement of binder = displacement of particle at boundary
- Newton's second law: stresses integrated over particle surface produce acceleration

Numerical Solution parameters:

- 1-µm wave amplitude
- 500-µm HMX particle
- Sylgard binder
- 500-kHz excitation frequency



Simplified diagram of single-particle embedded in a viscoelastic binder

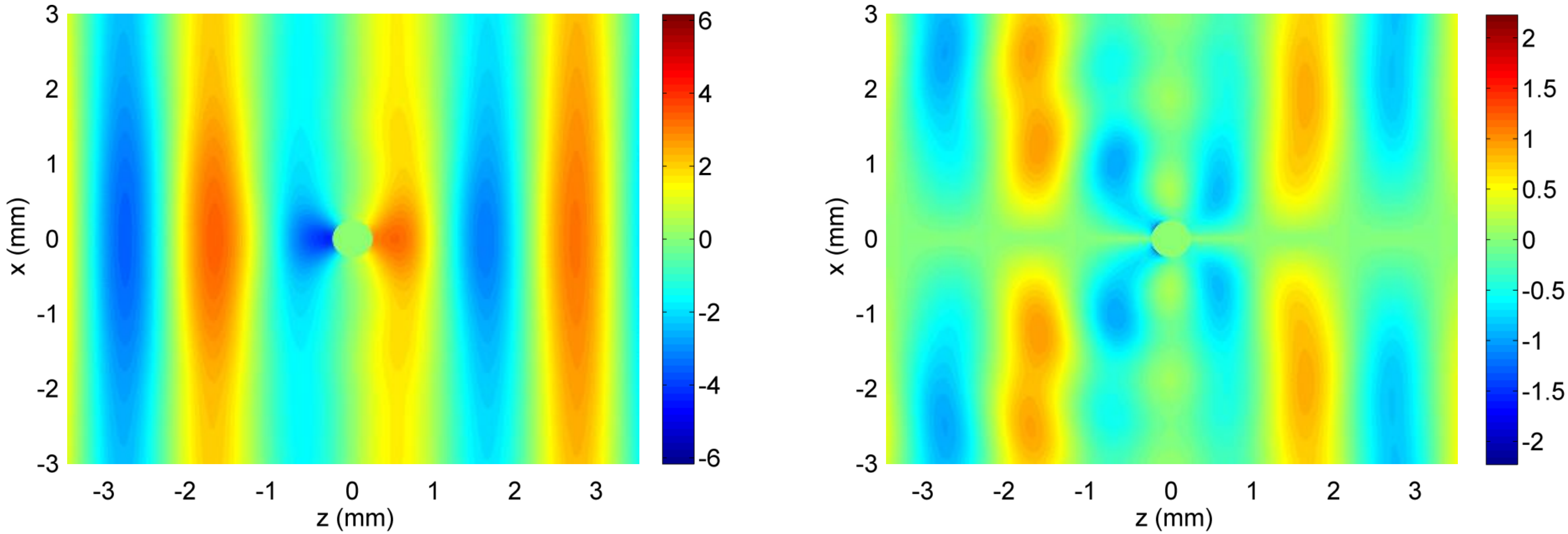
Mares, et.al., IMECE 2016

Stress Solution

- Solved by Pao and Mao in 1963 for linear elastic binder
- Expanded to lossy viscoelastic binder by Gaunard and Uberall in 1978
- Solved for lossy inclusion by Hinders, et. al. in 1994
- Solved with FE simulation by Chervinko in 2007

Real component of radial stress: $\Re(\tilde{\sigma}_{rr})$

Real component of shear stress: $\Re(\tilde{\sigma}_{r\theta})$

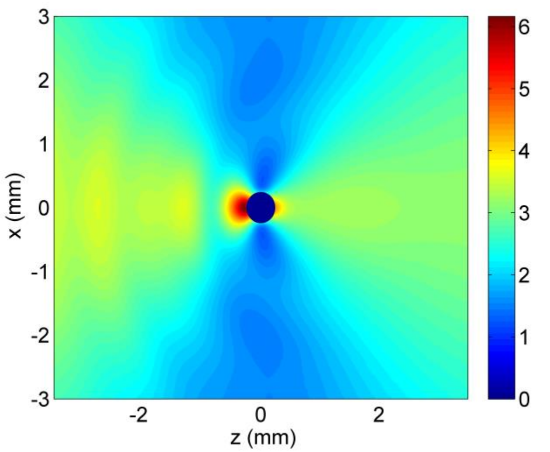


1-µm, 500-kHz harmonic plane wave excitation using Gaunard and Uberall expressions

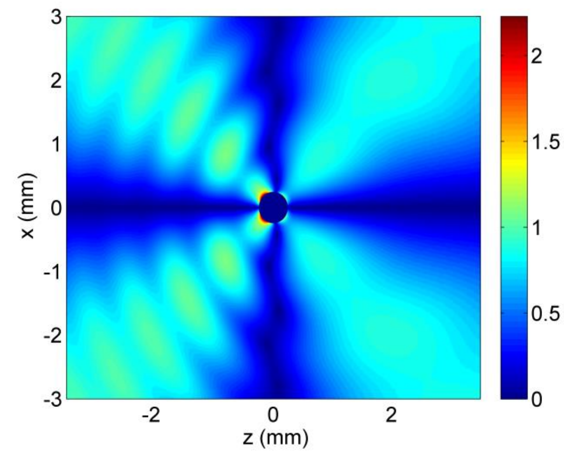
Periodic Excitation of a Single Spherical Particle

- **1-μm**, 500-kHz harmonic plane wave excitation
- 500-μm diameter HMX crystal in Sylgard

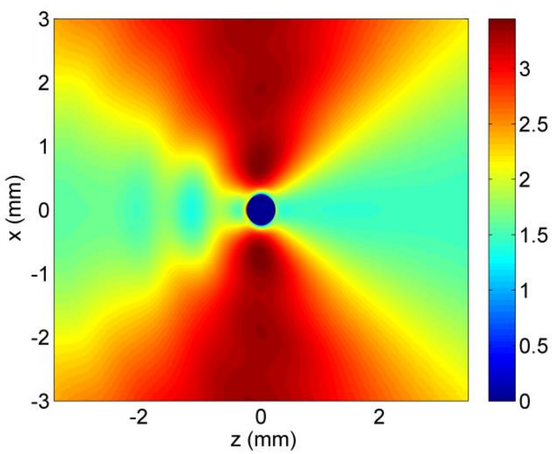
Radial Stress, $|\tilde{\sigma}_{rr}|$ (MPa)



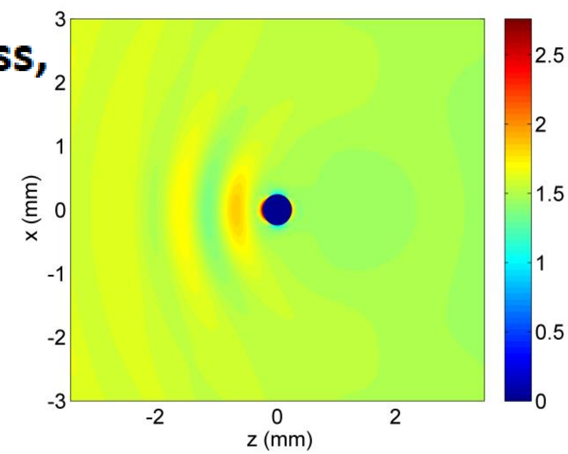
Shear Stress, $|\tilde{\sigma}_{r\theta}|$ (MPa)



"Polar" Stress, $|\tilde{\sigma}_{\theta\theta}|$ (MPa)



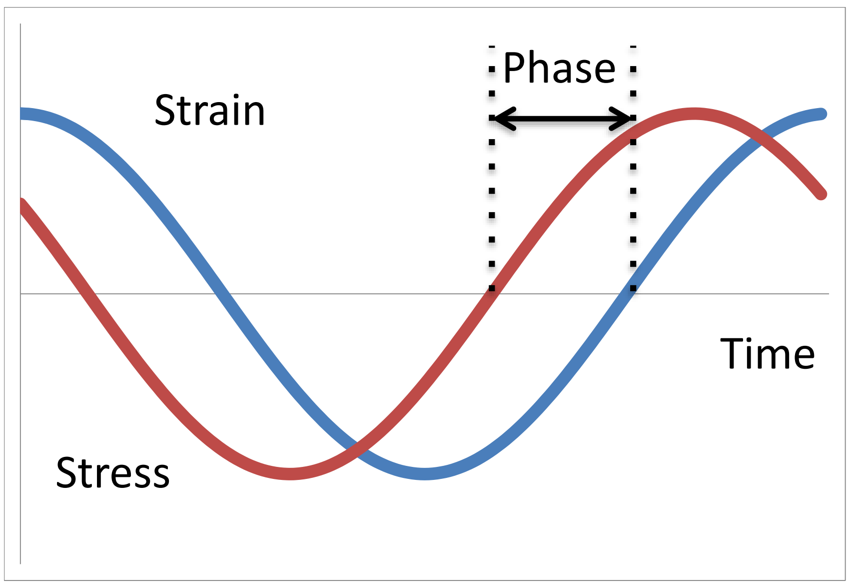
Azimuthal Stress, $|\tilde{\sigma}_{\phi\phi}|$ (MPa)



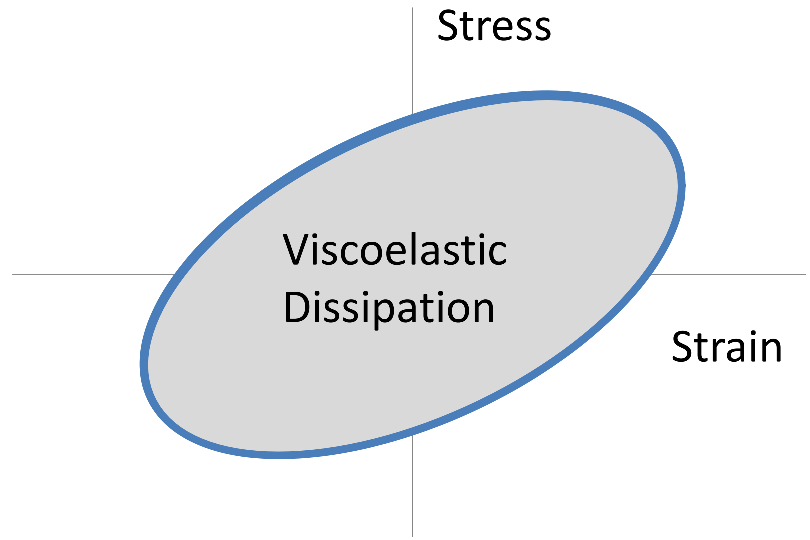
Viscoelastic Heating Model

- Based on losses in strain energy density per cycle of applied harmonic stress (hysteretic damping)

Single cycle of viscoelastic stress and strain



Phase plot of single cycle



Time-averaged heat generation (W/m^3):

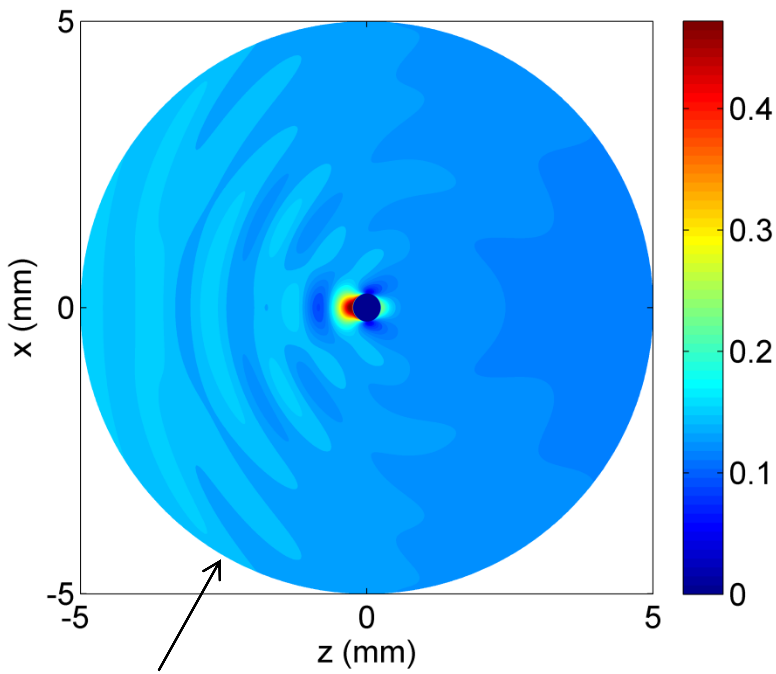
$$q = \frac{\omega}{2\pi}\int_{t_0}^{t_0+2\pi/\omega}\left(\sigma_{rr}\frac{\partial\varepsilon_{rr}}{\partial t} + \sigma_{\theta\theta}\frac{\partial\varepsilon_{\theta\theta}}{\partial t} + \sigma_{\phi\phi}\frac{\partial\varepsilon_{\phi\phi}}{\partial t} + 2\sigma_{r\theta}\frac{\partial\varepsilon_{r\theta}}{\partial t} + 2\sigma_{r\phi}\frac{\partial\varepsilon_{r\phi}}{\partial t} + 2\sigma_{\theta\phi}\frac{\partial\varepsilon_{\theta\phi}}{\partial t}\right)dt$$

Heat Generation in HMX-Sylgard System

Fourier's law of conduction:

$$r_m c_{p,m} = k_m \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin q}\frac{\partial}{\partial q}\left(\sin q \frac{\partial T}{\partial q} \right) \right] + q_m$$

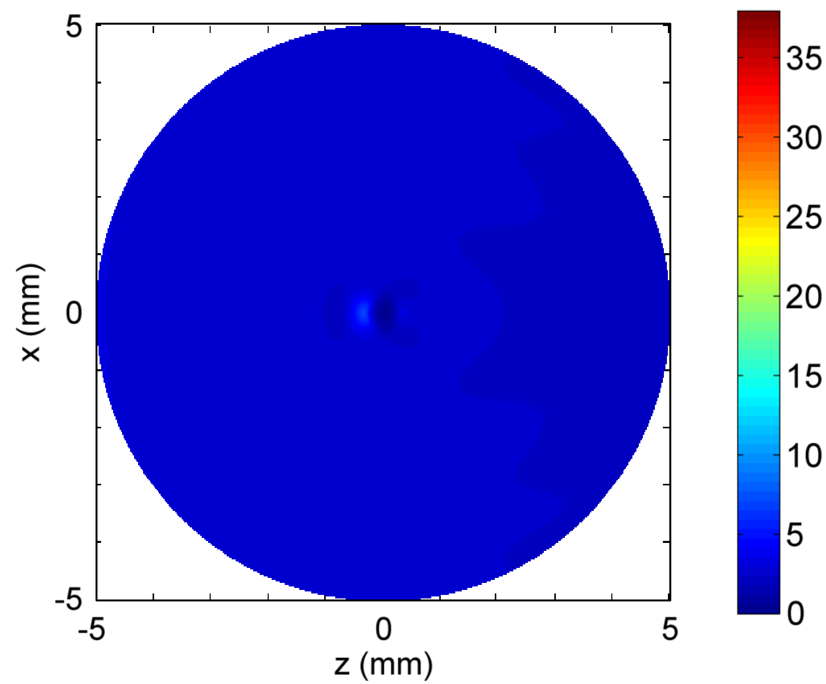
Time-averaged Heat Generation (W/mm³)



For the temperature solution, a free convective surface condition was applied at a large outer radius

1-µm, 500-kHz harmonic plane wave excitation

Temperature Increases (°C) from 0.05 to 0.5 s

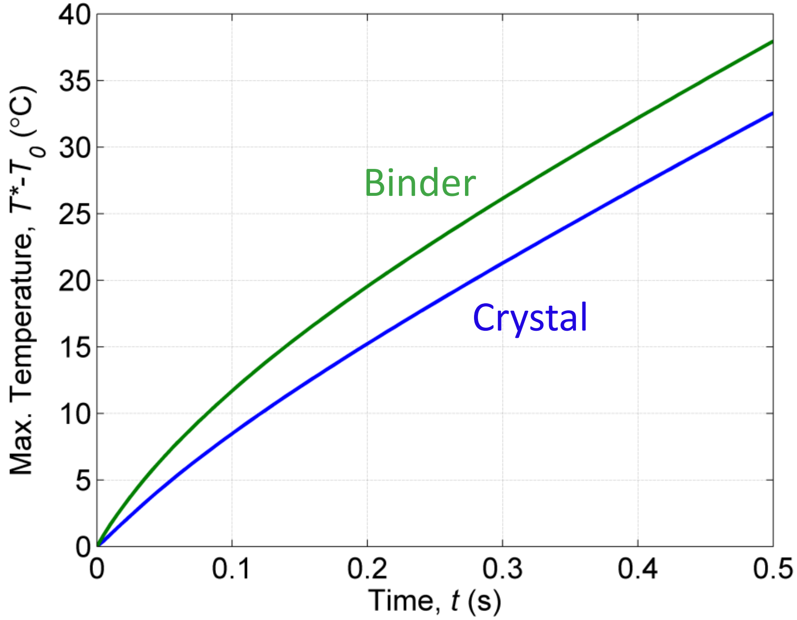


Animation shows 0.05 s increments, with one frame shown per second

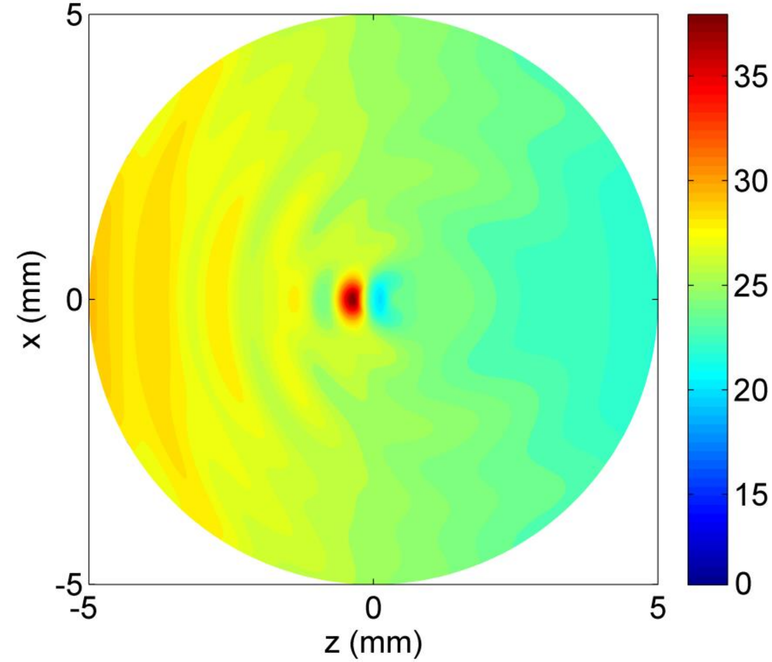
Temperature Increase in HMX-Sylgard System

- **1-μm**, 500-kHz harmonic plane wave excitation

Transient Max. Temperature Increase of Crystal and Binder

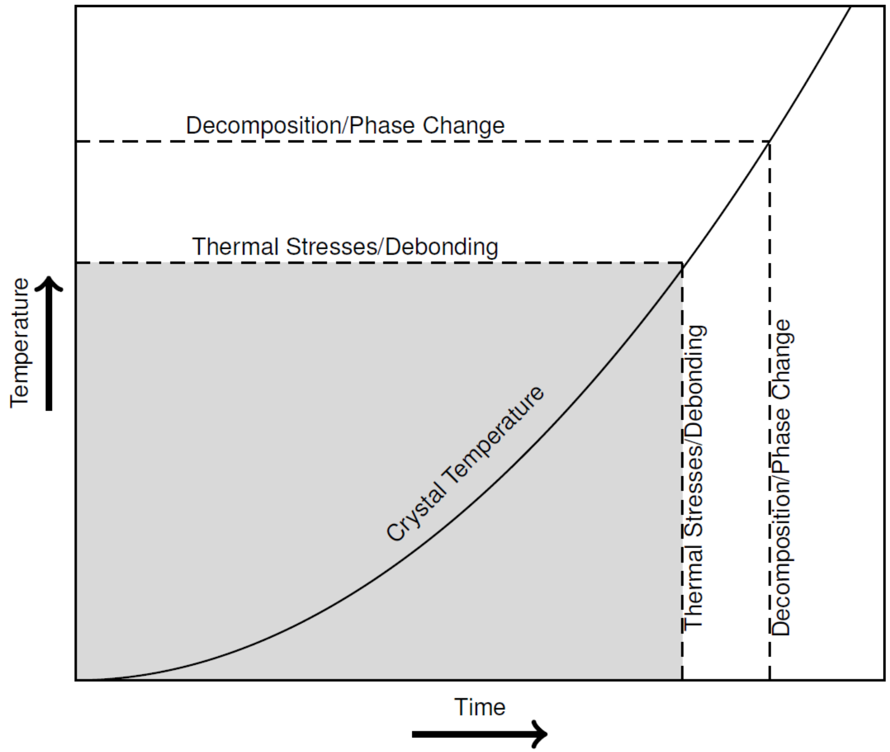


Temperature Distribution (°C) at t = 0.5 s

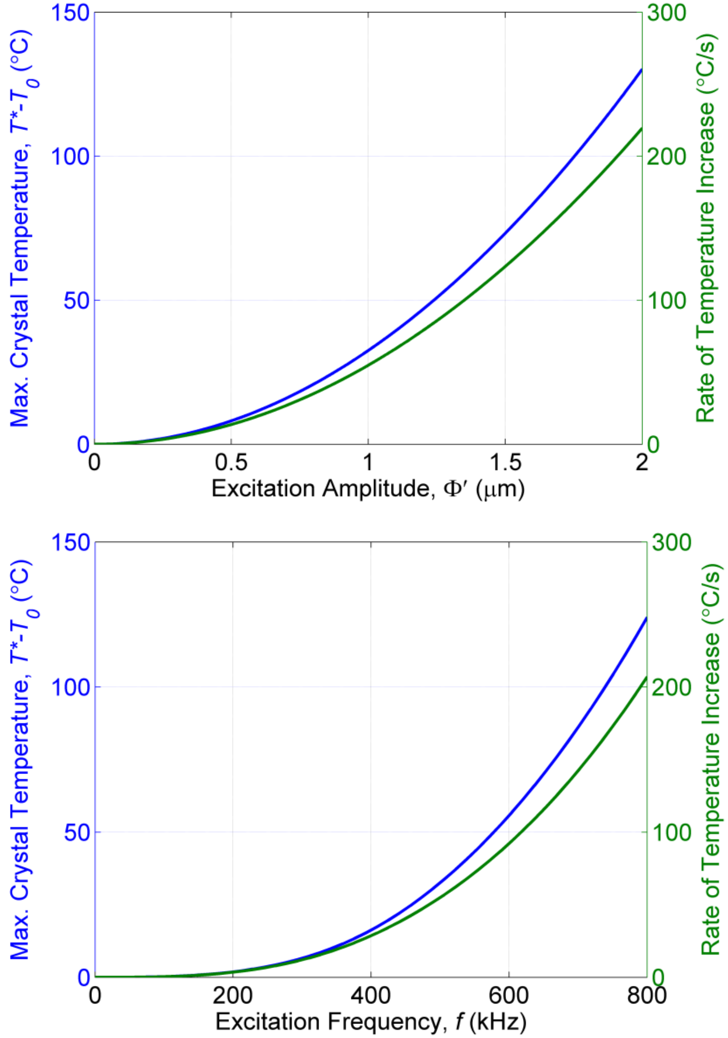


Compares well to Mares, et. al. (2014) in which heating rate were estimated to be between 37 to 125°C/s depending on shape, size, and identity of inclusion

Future Modeling Efforts



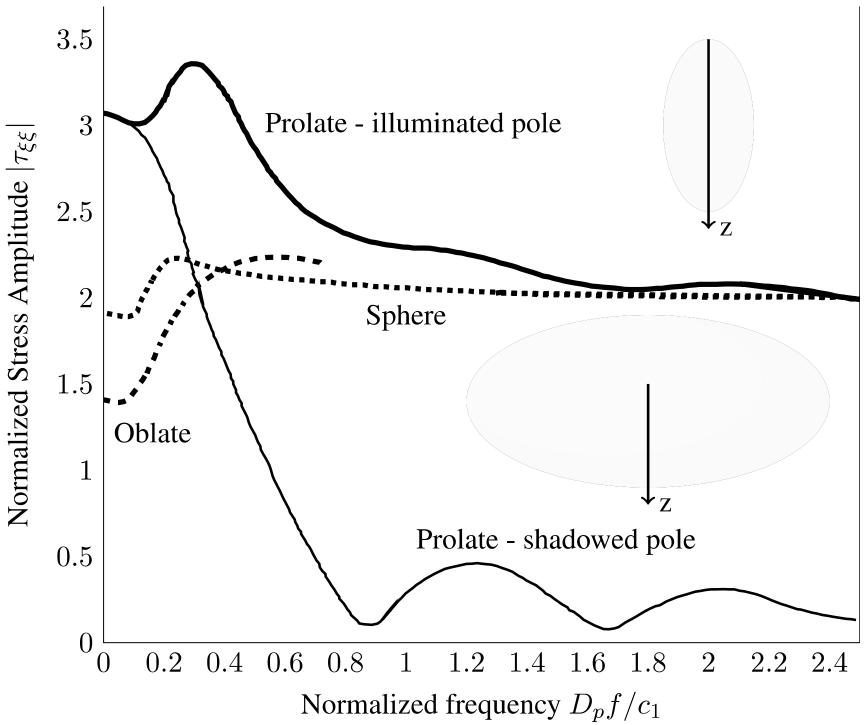
Mares et al., J. Appl. Mech., 2016 (Submitted).

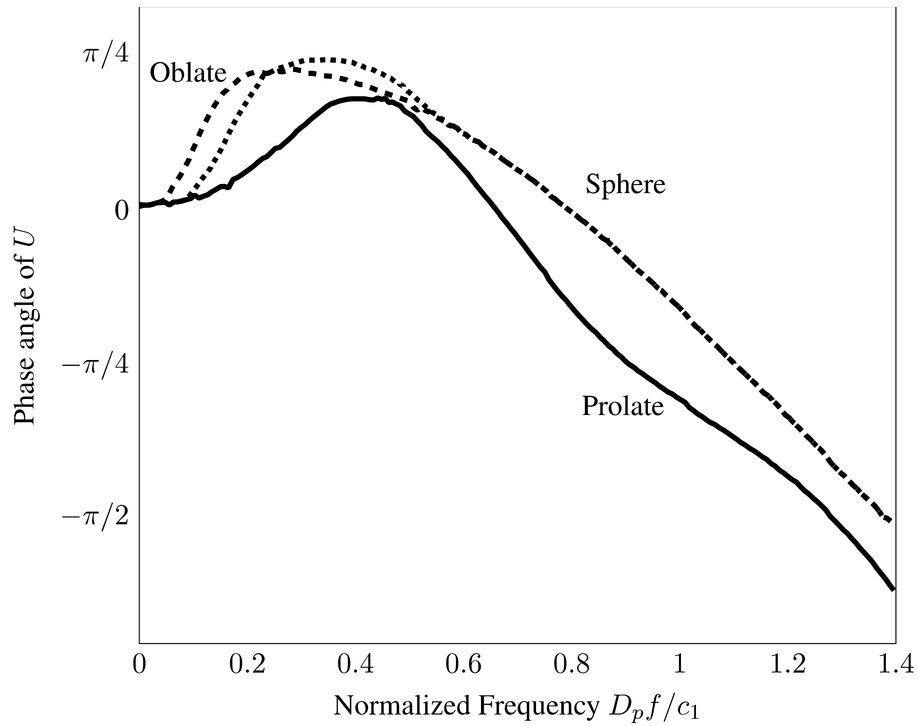


- Effect of temperature-dependent parameters
- Non-linear viscoelasticity
- Thermal stress effects
- Debonding effects
- Effect of binder and particle properties

Future modeling efforts: Particle morphology

Adapted from Oien, 1973





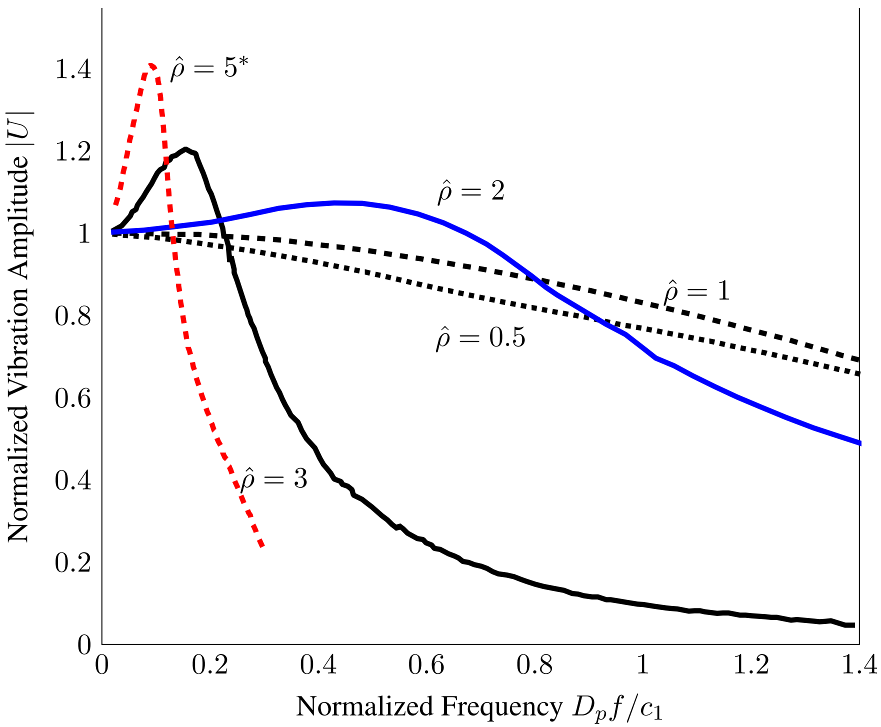
- Particle size and shape have a significant effect on stress amplitudes
- Relationship between frequency and particle size affects phase also
- Denser particle has larger vibrational amplitude

Questions?

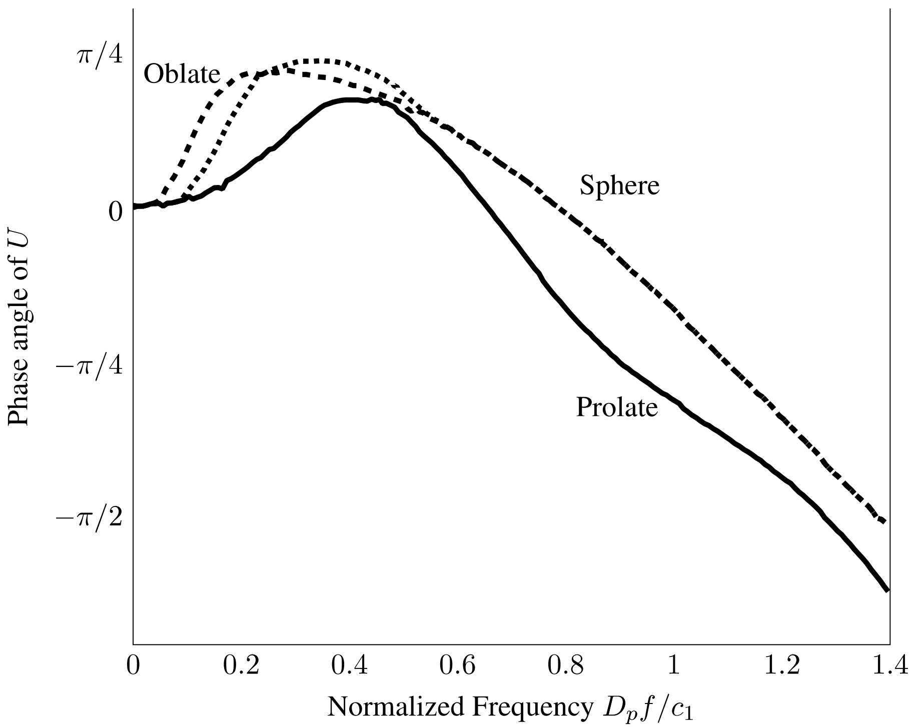
System dynamics

Particle motion described by Newton's second law:

$$\frac{4\pi a^3}{3}\rho\ddot{U} = \iint \left(\sigma_{rr}\cos\theta - \sigma_{r\theta}\sin\theta\right)a^2 \sin\theta\, d\theta\, d\varphi\Big|_{r=a}$$



Particle density affects vibration amplitude



Thermal Analysis Boundary Conditions

$$k_2 \frac{\partial T}{\partial r}(0,\theta,t) = -k_2 \frac{\partial T}{\partial r}(0,\theta+\pi,t),$$

$$T(a^-,\theta,t) = T(a^+,\theta,t),$$

$$k_2 \frac{\partial T}{\partial r}(a^-,\theta,t) = k_1 \frac{\partial T}{\partial r}(a^+,\theta,t),$$

$$k_1 \frac{\partial T}{\partial r}(R,\theta,t) = U_0 [T_0 - T(R,\theta,t)],$$

$$k_m \frac{\partial T}{\partial \theta}(r,0,t) = 0,$$

$$k_m \frac{\partial T}{\partial \theta}(r,\pi,t) = 0,$$