

Research of Exothermic Nanolaminates and their Structure-Property Relationships



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Problem

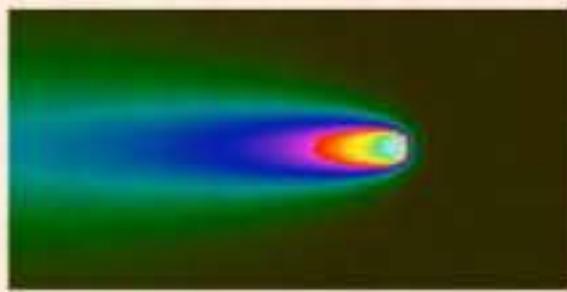
Although exothermic nanolaminate foils show potential as local heat sources, the scientific community does not fully understand the structure-property relationships of these materials.

Approach

Approach (Experiment and Modeling):

Research of ignition thresholds:
global and local stimulus
effects of pulse duration

Studies of reaction dynamics
and transient behaviors:
high-speed photography (micrometer/microsecond scales)
dynamic transmission electron microscopy (nanometer/nanosecond scales)



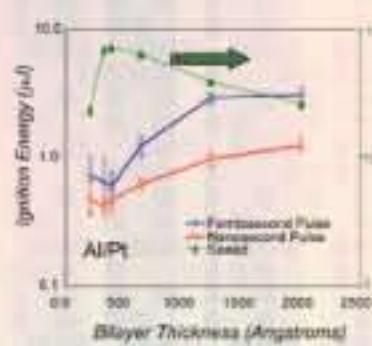
Investigation of aging:
kinetics, loss of stored chemical energy

Examine the properties of transformed multilayers:
heat output, optical, magnetic

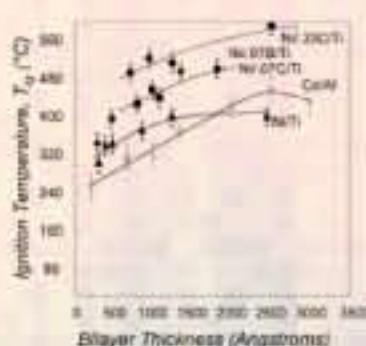
* Acknowledge: T. Lagrange LLNL

Experimental Studies of Ignition

Localized Ignition:
Threshold influenced
by bilayer design,
pulse length



Global Heating:
 $T_{ig} < T_m$ (constituents)



Studies of Self-Propagating Reactions

Oscillating reaction front probed on the microsecond scale
Example: Co/Al



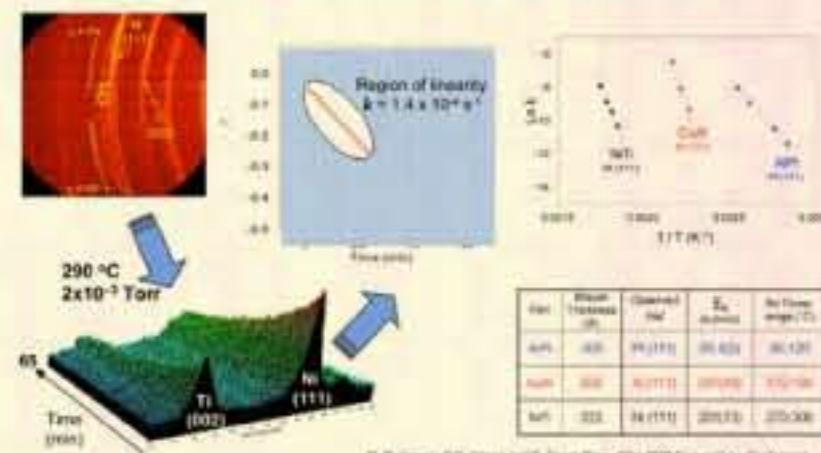
Times shown are relative to initial foil ignition
Heat direction

Phase evolution on the nanosecond scale



* Acknowledge: T. Lagrange, J. Kim, LLNL

Accelerated Aging of Exothermic Nanolaminates

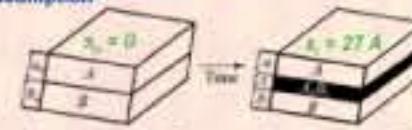


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Modeling Exothermic Nanolaminate Behaviors

1D diffusion controlled growth reaction
with zero strain assumption*



ODEs

$$\frac{dx}{dt} = -\frac{D_A}{\rho_A}$$

$$\frac{dx}{dt} = \frac{D_B}{\rho_B}$$

$$\frac{dx}{dt} = -\frac{D}{\rho} \left(1 + \frac{b}{\rho} \right)$$

$$\frac{dx}{dt} = -\frac{D}{\rho} \left(1 + \frac{b}{\rho} \right)$$

$$D = D_0 \exp(-\frac{x}{L})$$

$$a = \frac{\rho_A D_A}{\rho_A D_A + \rho_B D_B}$$

$$b = a \frac{\rho_B D_B}{\rho_A D_A + \rho_B D_B}$$

$$\rho_{AB} = \frac{\rho_A D_A + \rho_B D_B}{\rho_A + \rho_B}$$

*S. H. Adachi et al. "Propagation of ignition reaction in metal-metall multilayer," *Journal of Heat Transfer*, Vol. 121, pp. 2748-2753.

Auxiliary Eqns.

$$D = D_0 \exp(-\frac{x}{L})$$

$$a = \frac{\rho_A D_A}{\rho_A D_A + \rho_B D_B}$$

$$b = a \frac{\rho_B D_B}{\rho_A D_A + \rho_B D_B}$$

$$\rho_{AB} = \frac{\rho_A D_A + \rho_B D_B}{\rho_A + \rho_B}$$

Algorithm

Choose ρ_{AB} , calculate ρ_A

Choose x_s , calculate ρ_B , L , and F

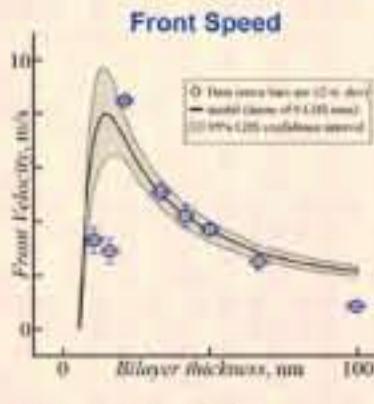
Solve ODEs for x and F

Energy Equation

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (\lambda \nabla T) = -\rho \dot{P} \frac{\partial P}{\partial t}$$

Modeling the Steady-State Reaction Rates of Exothermic Nanolaminates

Example: Co/Al

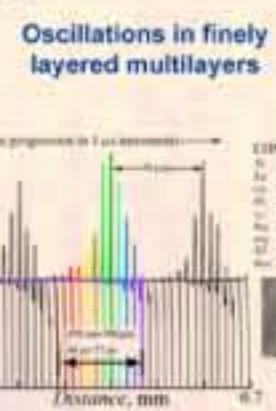
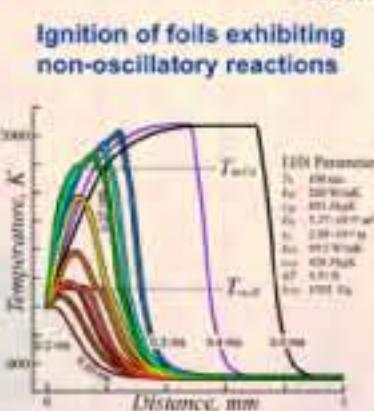


Uncertainty Parameters



Predicting Transient Temperature Profiles

Example: Co/Al



M. Hobbs, S. Adachi and J.P. McDaniel, *Proc. of the 10th Int'l Conf. on Adv. Computational Methods and Exp. Measurements in Heat Transfer* 2008

Significance

Fundamental:

- Improved understanding of ignition
- Improved understanding of the dynamics of high-rate reactions
 - morphology evolution
 - phase formation (includes metastable phases),
 - oscillatory behaviors
 - effects of boundary conditions
- Discovery of new exothermic systems
- Predictive modeling of reactions in metal-metal systems
- Assessment of aging (shelf life)

Potential new applications:

- Sensors/actuators
- Power systems
- Improved joining processes

