

Research of Exothermic Nanolaminates and their Structure-Property Relationships



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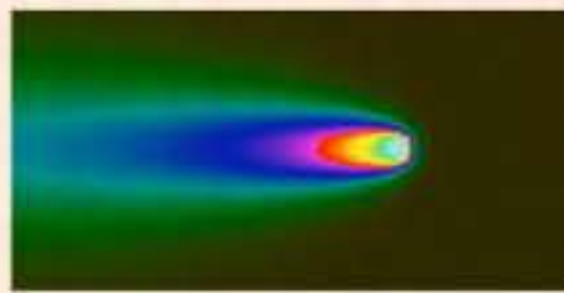
Problem

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:

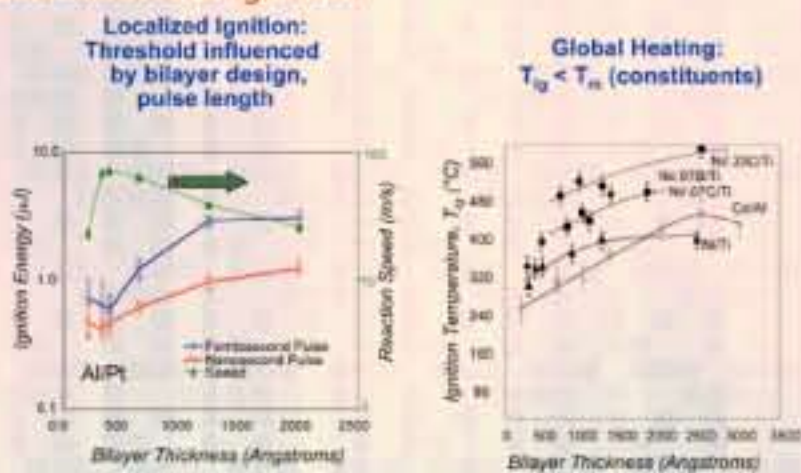
kinetics, loss of stored chemical energy

Examine the properties of transformed multilayers:

heat output, optical, magnetic

* Acknowledge: T. Lagrange LLNL

Experimental Studies of Ignition

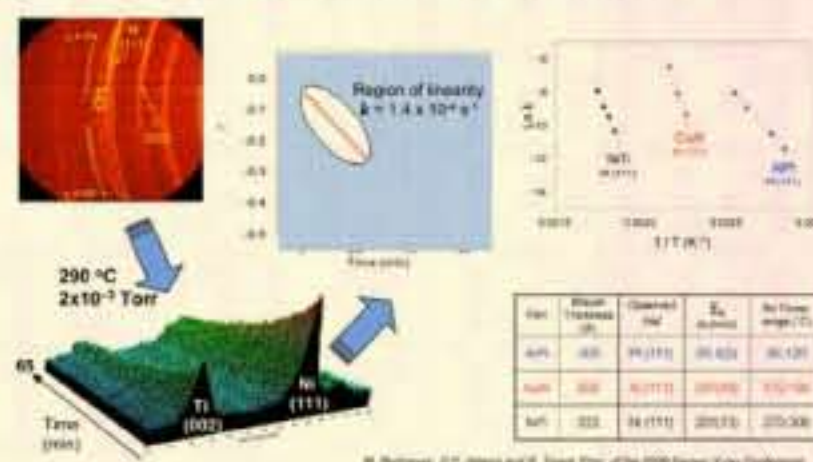


Studies of Self-Propagating Reactions



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

Accelerated Aging of Exothermic Nanolaminates



Modeling Exothermic Nanolaminate Behaviors

1D diffusion controlled growth reaction with zero strain assumption*



ODEs

$$\frac{d\xi_A}{dt} = -\frac{D}{l} \frac{d\xi_A}{dx}$$

$$\frac{d\xi_B}{dt} = -\frac{D}{l} \frac{d\xi_B}{dx}$$

$$\frac{d\xi}{dt} = -\frac{D}{l} \left(1 + \frac{\xi_A}{\xi_B}\right) \frac{d\xi}{dx}$$

$$\frac{dT}{dt} = -\frac{D}{l} \frac{dT}{dx}$$

Auxiliary Eqns.

$$D = D_0 \exp\left(-\frac{E_a}{RT}\right)$$

$$a = \frac{a_0 \exp(-E_a/RT)}{1 + \frac{\xi_A}{\xi_B} \frac{D_A}{D_B}}$$

$$h = a \frac{D_A \xi_A}{D_B \xi_B}$$

$$\rho_{AB} = \frac{\xi_A \xi_B}{\xi_A + \xi_B}$$

Algorithm

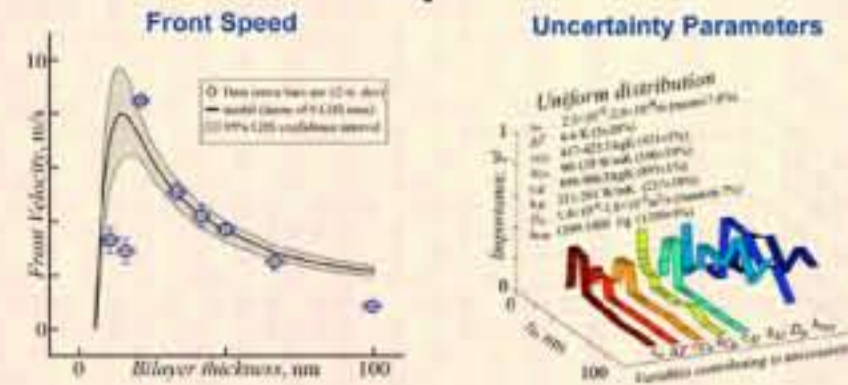
Choose x , calculate ξ ,
Choose x , calculate ξ , and T ,
Solve ODE's for ξ and T

Energy Equation

$$\rho \frac{dT}{dt} = \nabla \cdot (k \nabla T) - Q \frac{d\xi}{dt}$$

Modeling the Steady-State Reaction Rates of Exothermic Nanolaminates

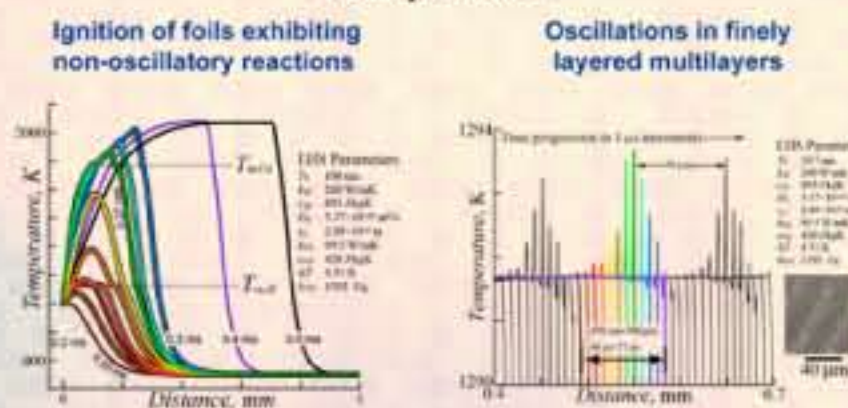
Example: Co/Al



D.P. Adams et al. J. Appl. Phys. 194, 2002
M. Hobbs, D. Adams and J.P. McDonald, Proc. of the 10th Int. Conf. on Adv. Computational Methods and Exp. Measurements in Heat Transfer 2008

Predicting Transient Temperature Profiles

Example: Co/Al



M. Hobbs, D. Adams and J.P. McDonald, Proc. of the 10th Int. 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