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Analytical modelling of propagation velocity in nanolaminates

In non-stoichiometric, shock impacted, and electron transparent systems

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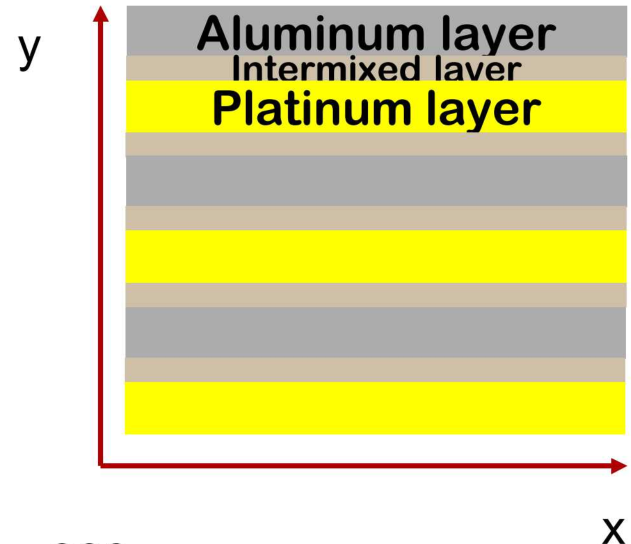
Video of Laser Ignition and Self-Propagating Reaction in Al/Pt Multilayer



760 W/cm^2
164 nm Bilayer, 31 m/s
1.8 µs per frame, played at 4 fps

300 µm

The relationship between physical parameters and propagation velocity

From Mann, Gavens, Reiss, Van Heerden, Bao, and Weihs, J. Appl. Phys. 1997:

Fick's Second Law

$$\frac{dC}{dt} - \nabla \cdot D\nabla C = 0$$

Heat Equation

$$c_p\rho\frac{dT}{dt} - c_p\rho\lambda\nabla^2 T = \frac{dQ}{dt}$$

Solved for the case of a moving wave

$$v_x^2 = \left(\sum_{n=odd}\frac{k_n^2}{\alpha_n^2}\right)^{-1}\frac{4\lambda_x^2 R T_f^2 D}{E_A\lambda_y(T_{ad}-T_0)}exp\left(\frac{-E_A}{RT_f}\right)$$

Values for model parameters are informed by experimental data

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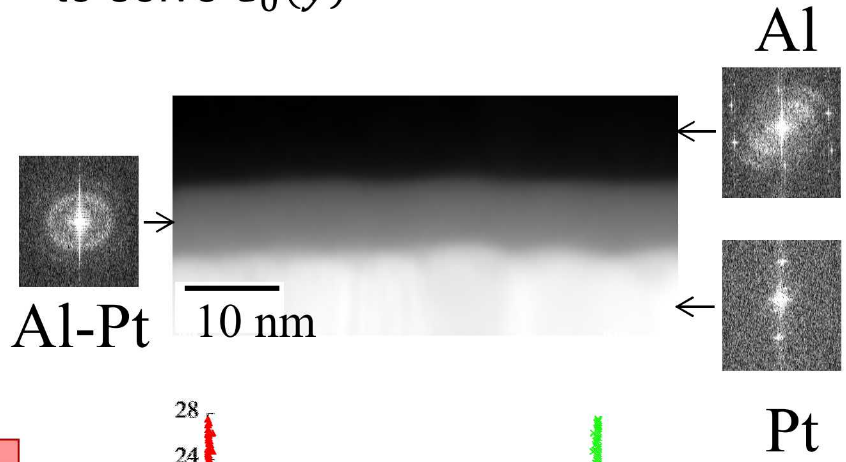
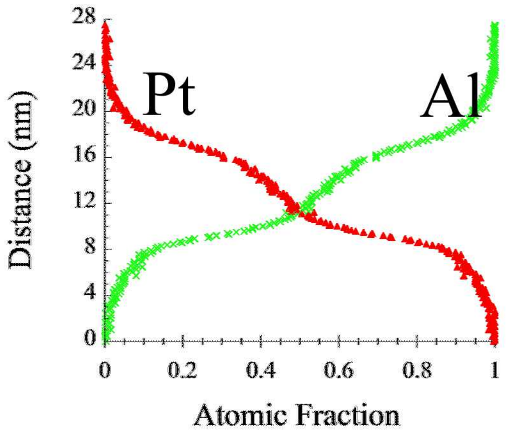
Concentration at each 1 Å wide mesh point comes from STEM-EDS to solve $C_0(y)$



Series of eigenvalues, α_n, and Fourier coefficients, k_n, account for the potential energy lost to premixed material as a function of initial concentration, $C_0(y)$, for quarter period δ.

$$\boxed{\alpha_n = \frac{n\pi}{2\delta} \qquad k_n = \frac{1}{2\delta}\int_{-2\delta}^{2\delta} C_0(y)\, sin(\alpha_n y) dy}$$



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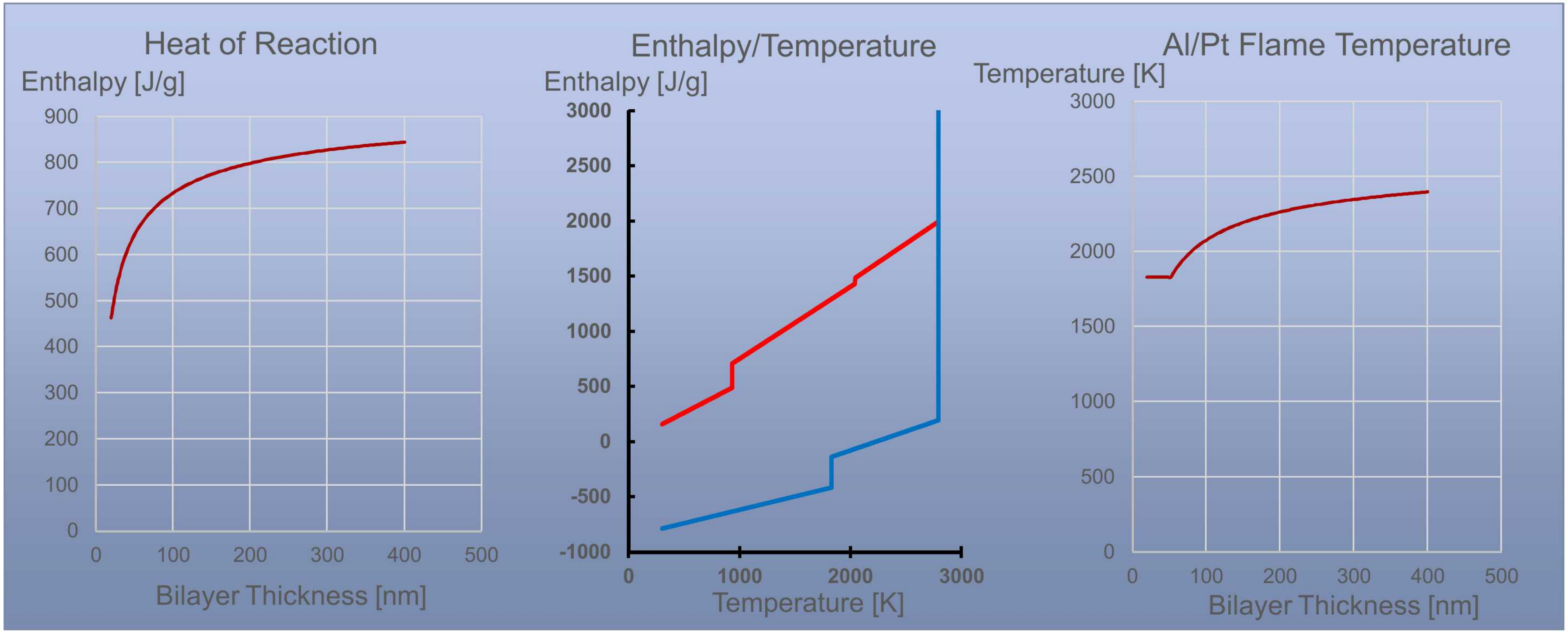
Heat of reaction from calorimetry and enthalpy-temperature diagrams allow for the calculation of adiabatic and flame temperatures



Thermal Conductivity in a three-parameter fit of velocity data

$$v_x^2 = \boxed{\left(\sum_{n=odd} \frac{k_n^2}{\alpha_n^2}\right)^{-1}} \frac{4\lambda_x^2 R T_f^2 D}{E_A \lambda_y (T_{ad} - T_0)} exp\left(\frac{-E_A}{R T_f}\right)$$

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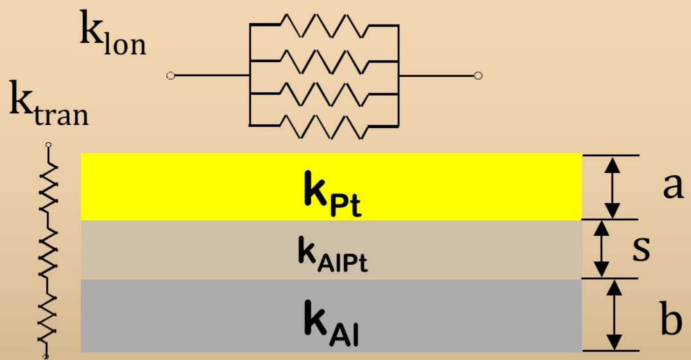
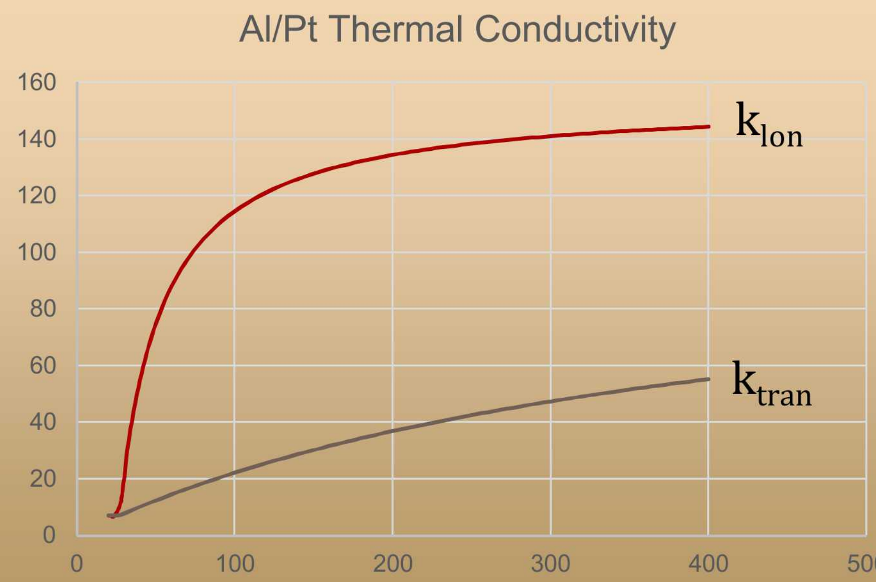


$$F = 1 - \frac{s}{a \cdot w} \qquad w = 1 + \frac{b}{a}$$

$$k_{tran}(t,T) = \left(\frac{F}{k_{Al}(T) \cdot w} + \frac{F(w-1)}{k_{Pt}(T) \cdot w} + \frac{1-F}{k_{AlPt}(T)}\right)^{-1}$$

$$k_{lon}(t,T) = \frac{k_{Al}(T)F}{w} + \frac{k_{Pt}(T)F(w-1)}{w} + k_{AlPt}(T)[1-F]$$



Pair of best fit for activation energy and diffusion coefficient

$$v_x^2 = \boxed{\left(\sum_{n=odd} \frac{k_n^2}{\alpha_n^2}\right)^{-1}} \frac{4\lambda_x^2 R T_f^2 D}{E_A \lambda_y (T_{ad} - T_0)} exp\left(\frac{-E_A}{R T_f}\right)$$

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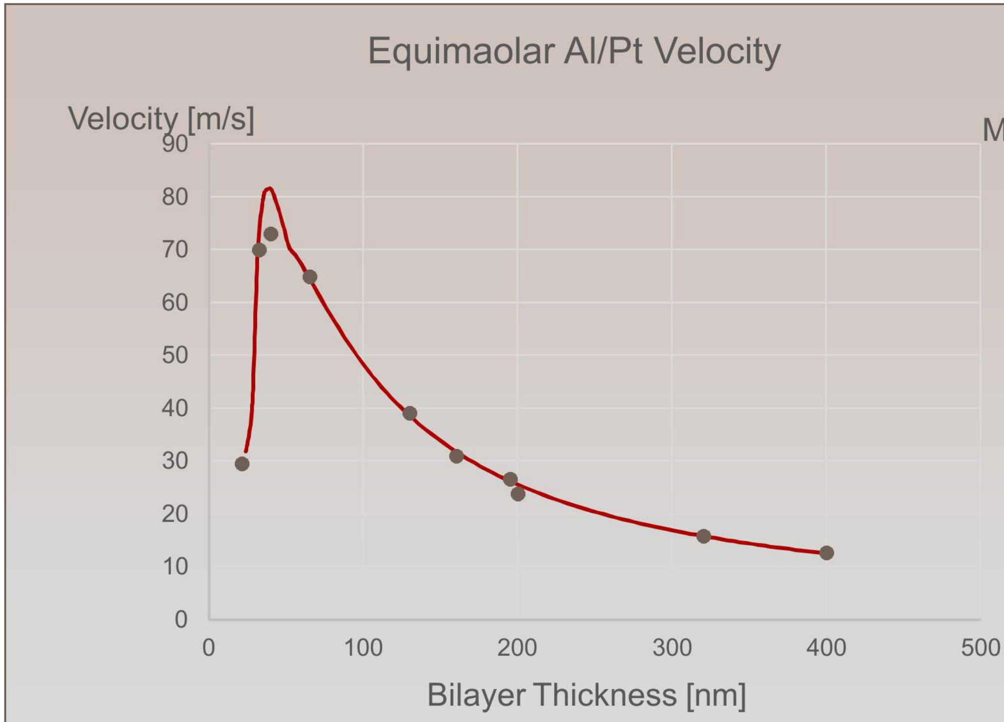
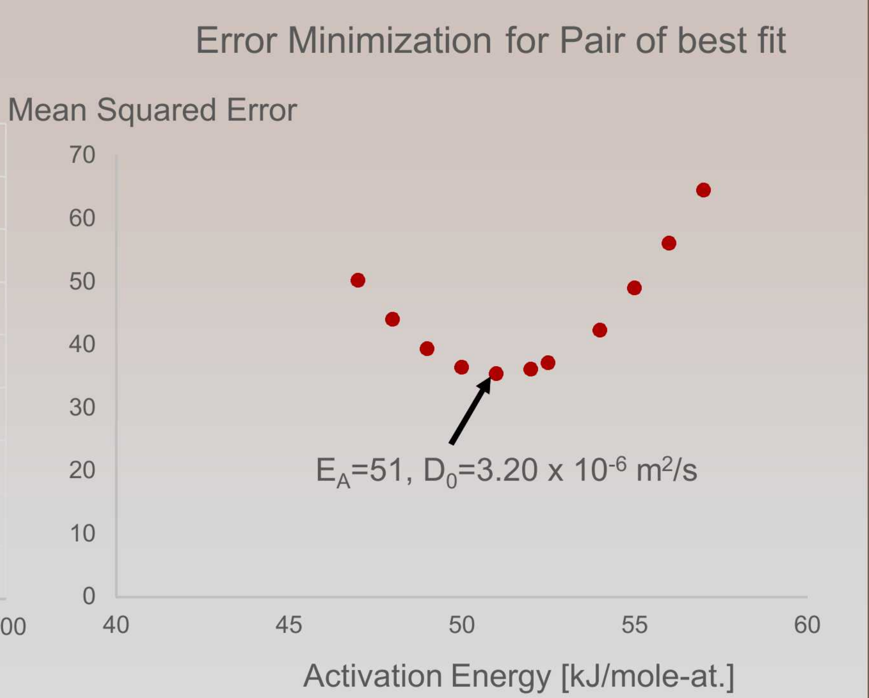
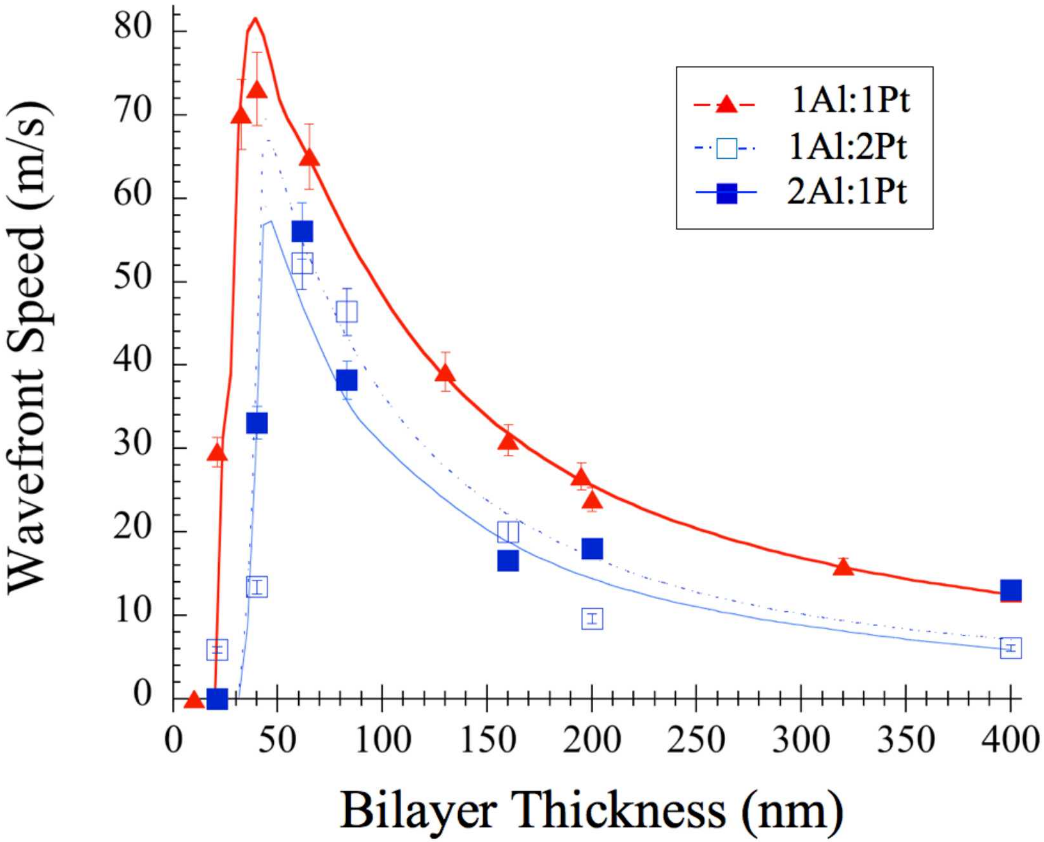
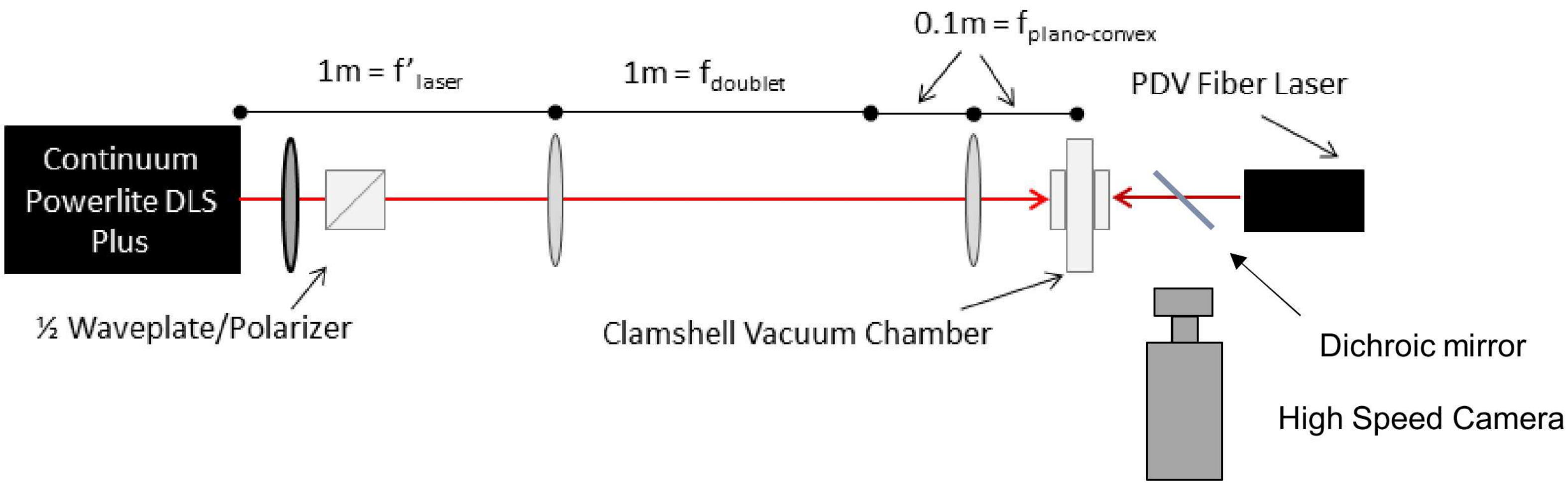


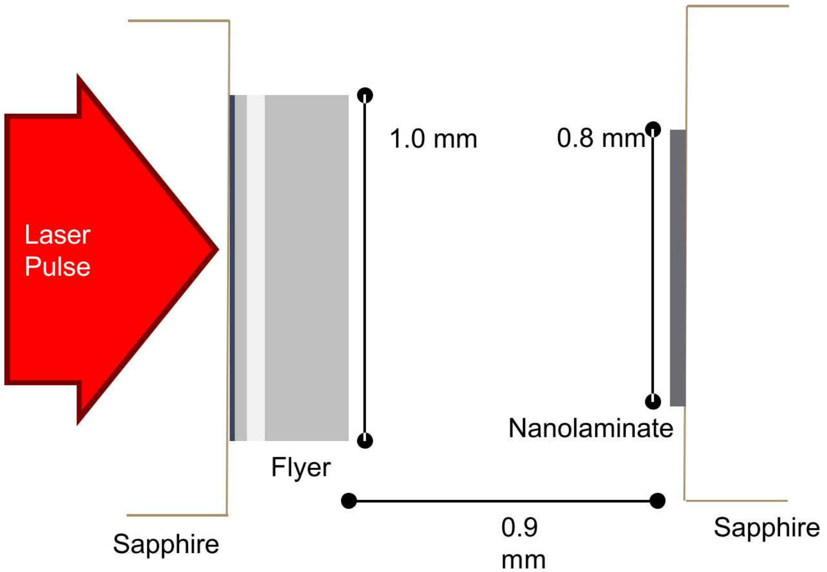


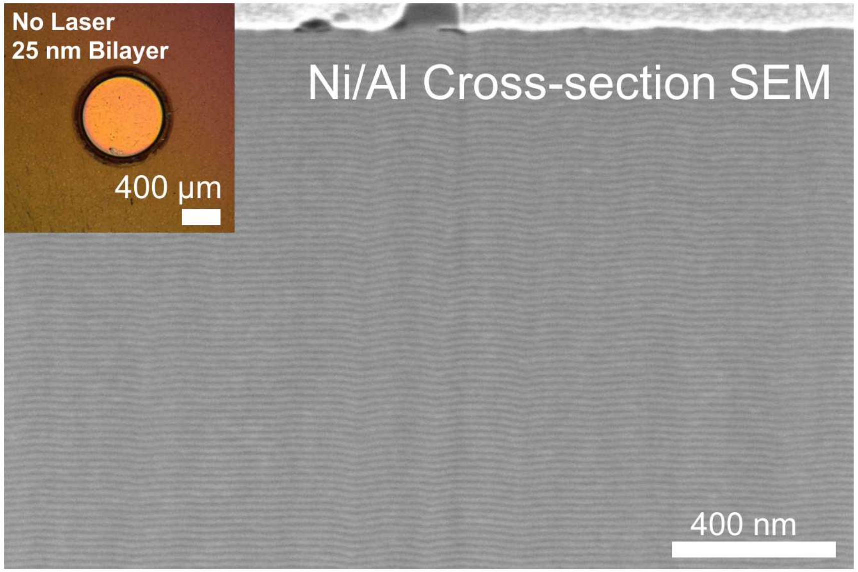
Material parameters remain constant for fitting off-stoichiometric compositions of Al/Pt



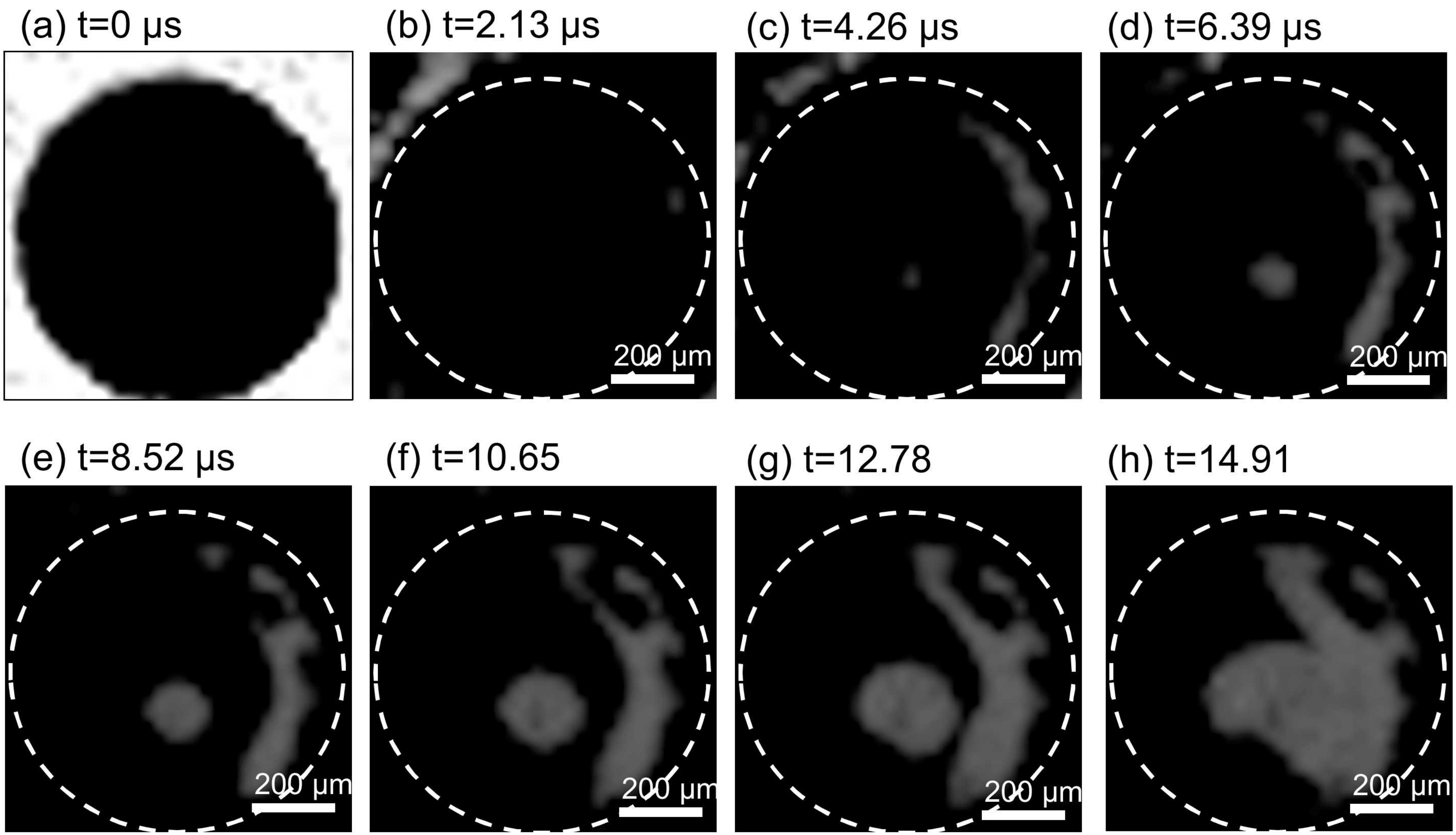
Laser flyer plate impact of Ni/Al



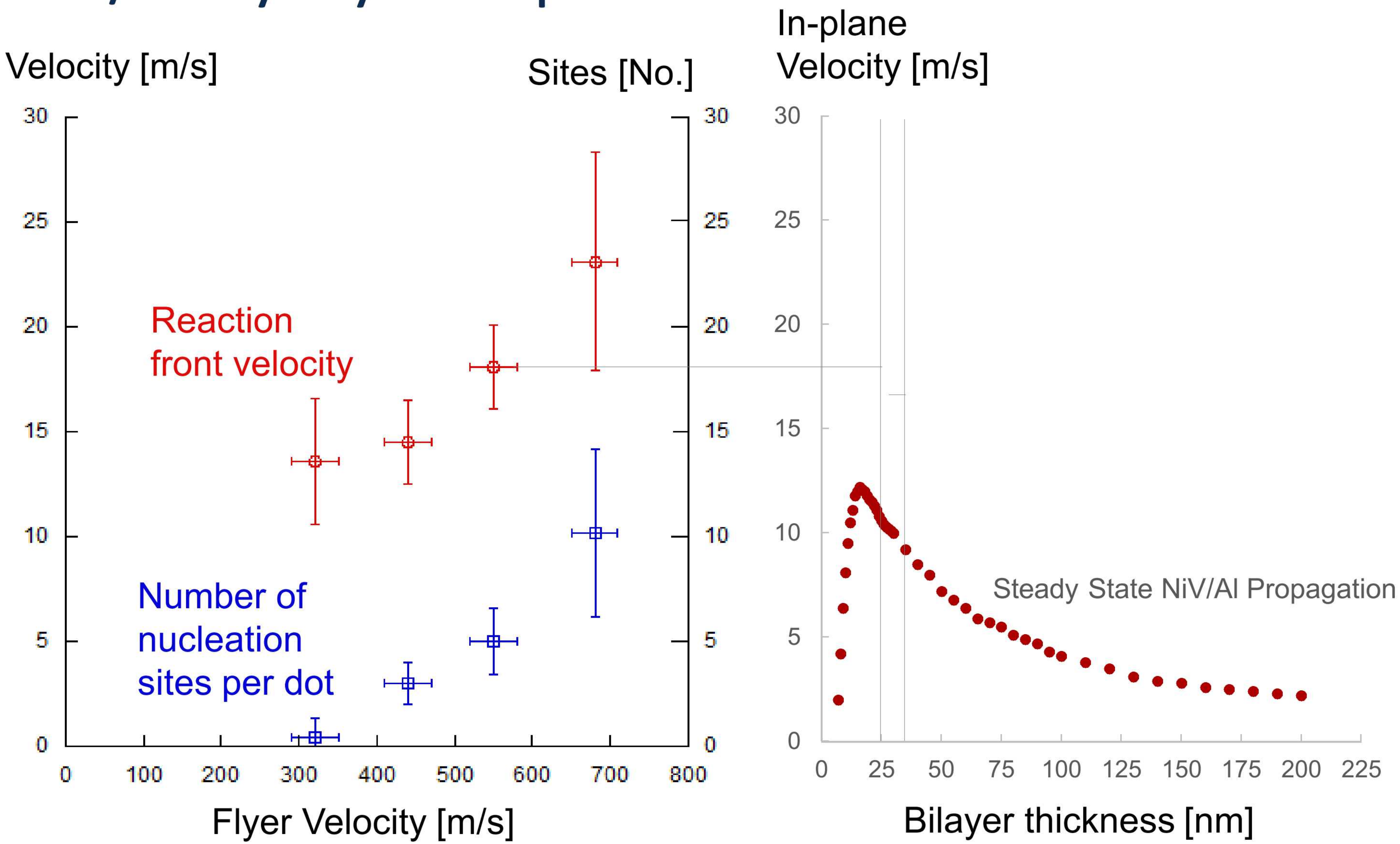




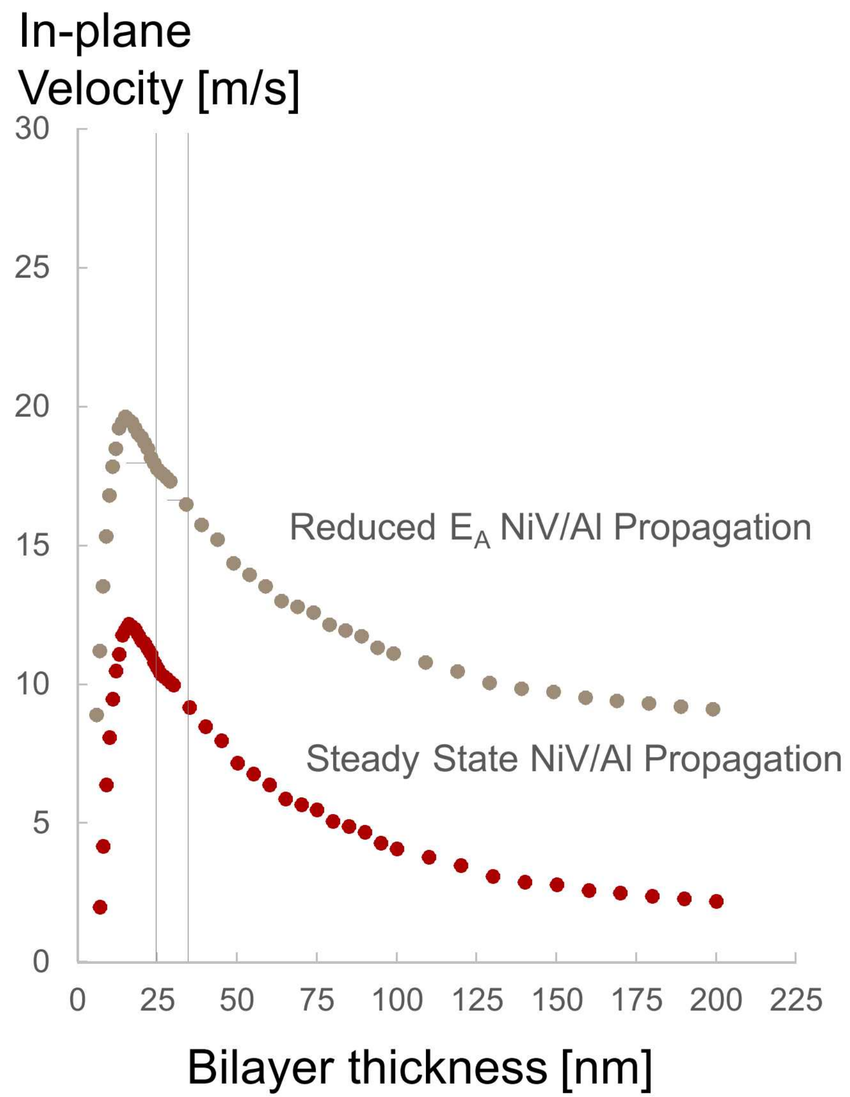
Videography of NiV/Al impact at 440 m/s

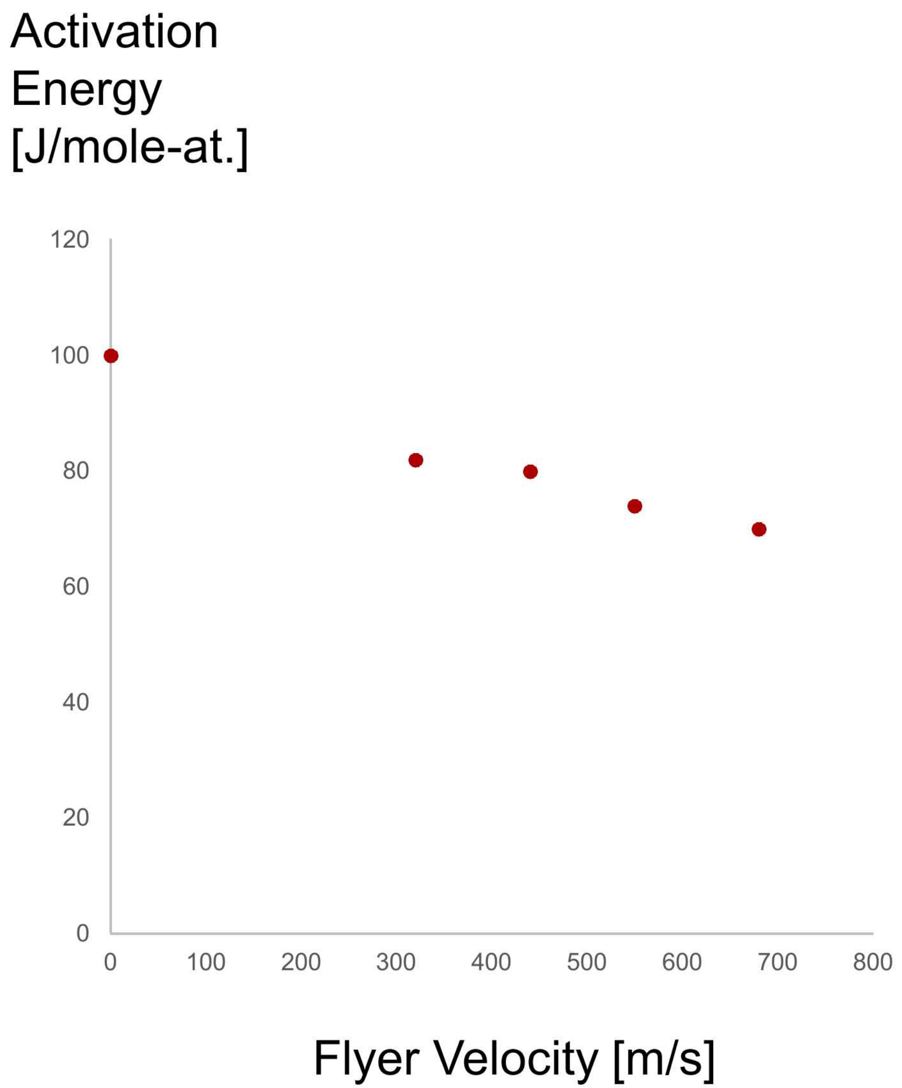


Reaction velocity of 25 nm Bilayer NiV/Al by Flyer Impact

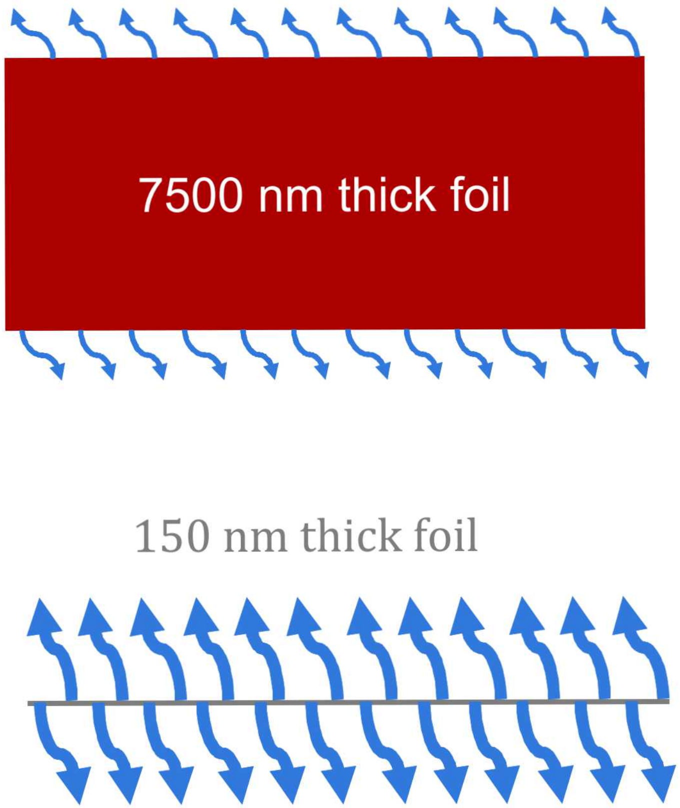


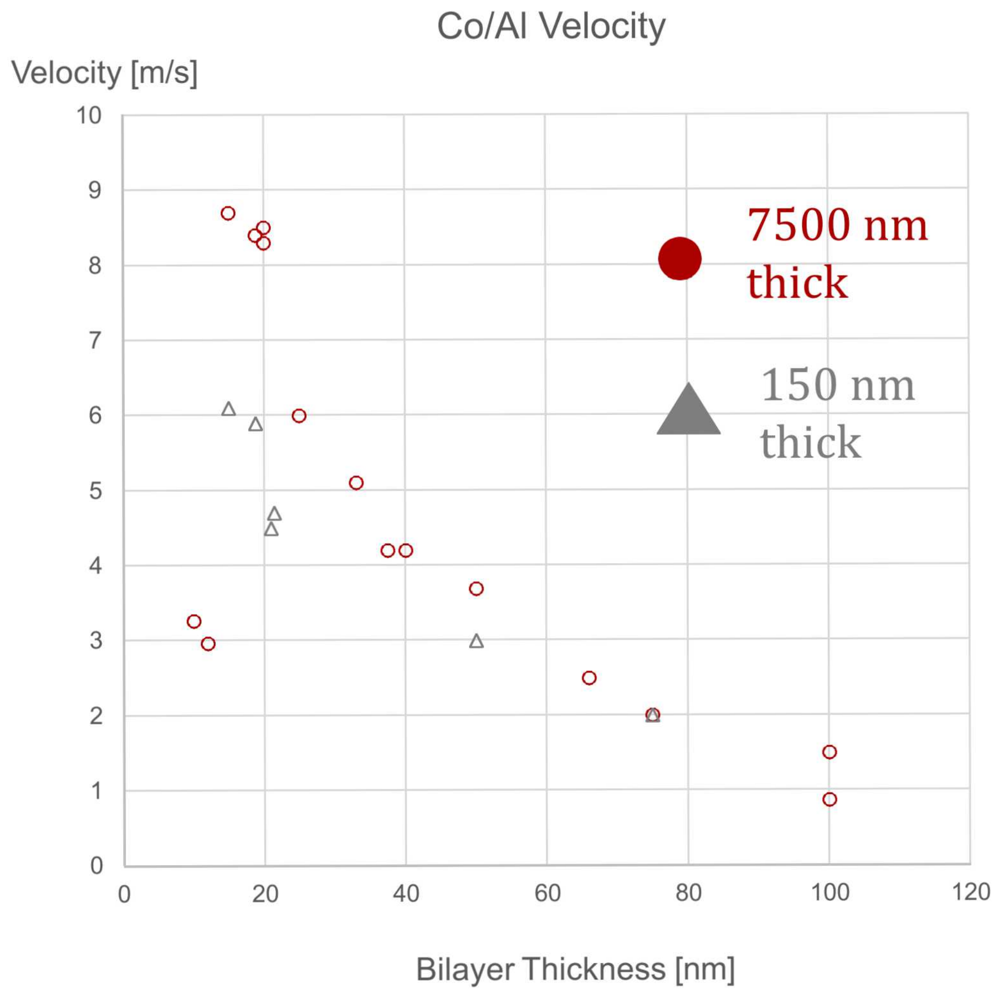
Reduction in Ni/Al Activation Energy after Impact





Radiation Loss in Electron Transparent Samples

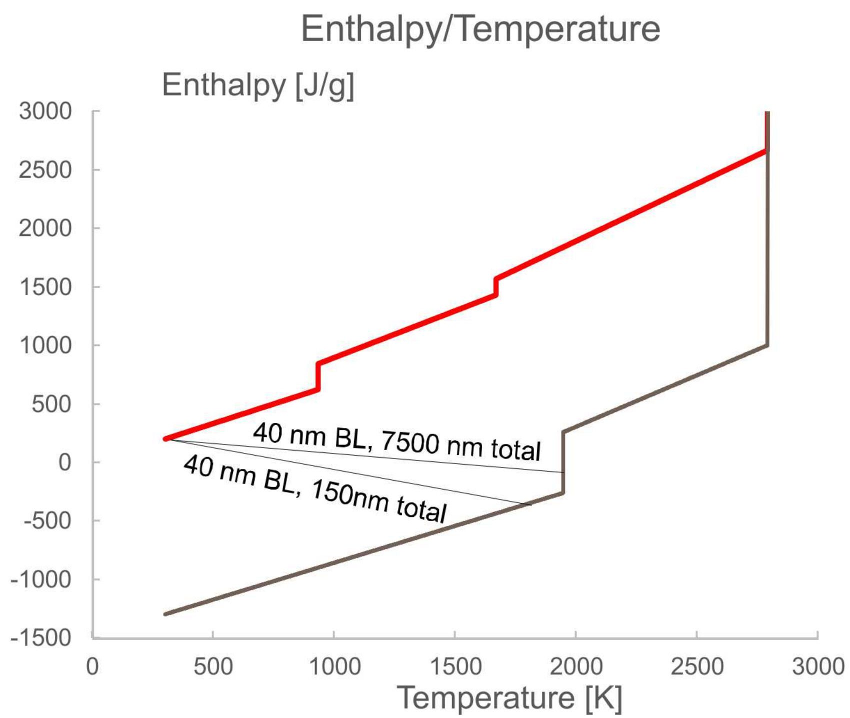


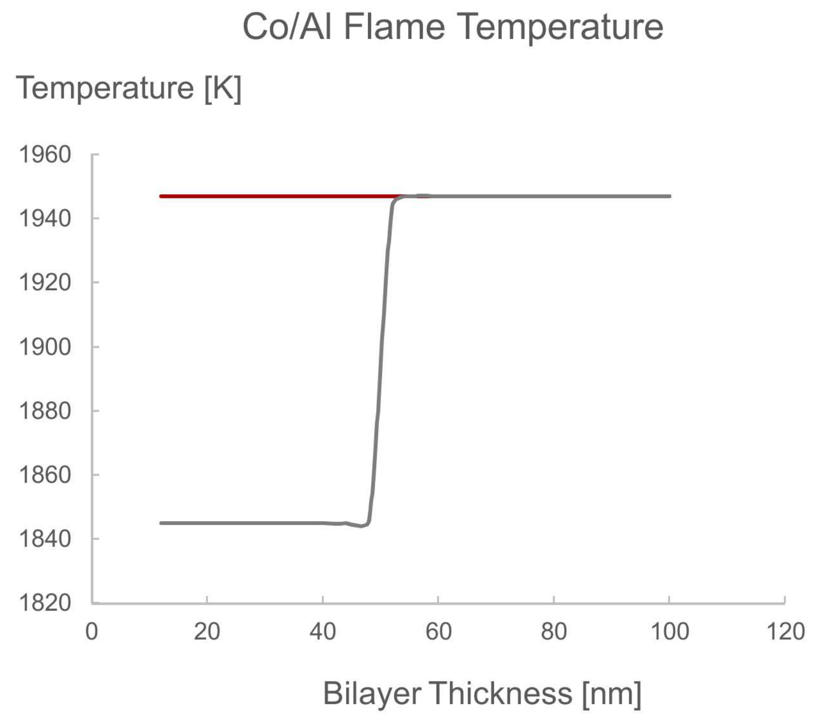


Accounting for Heat Loss in Model

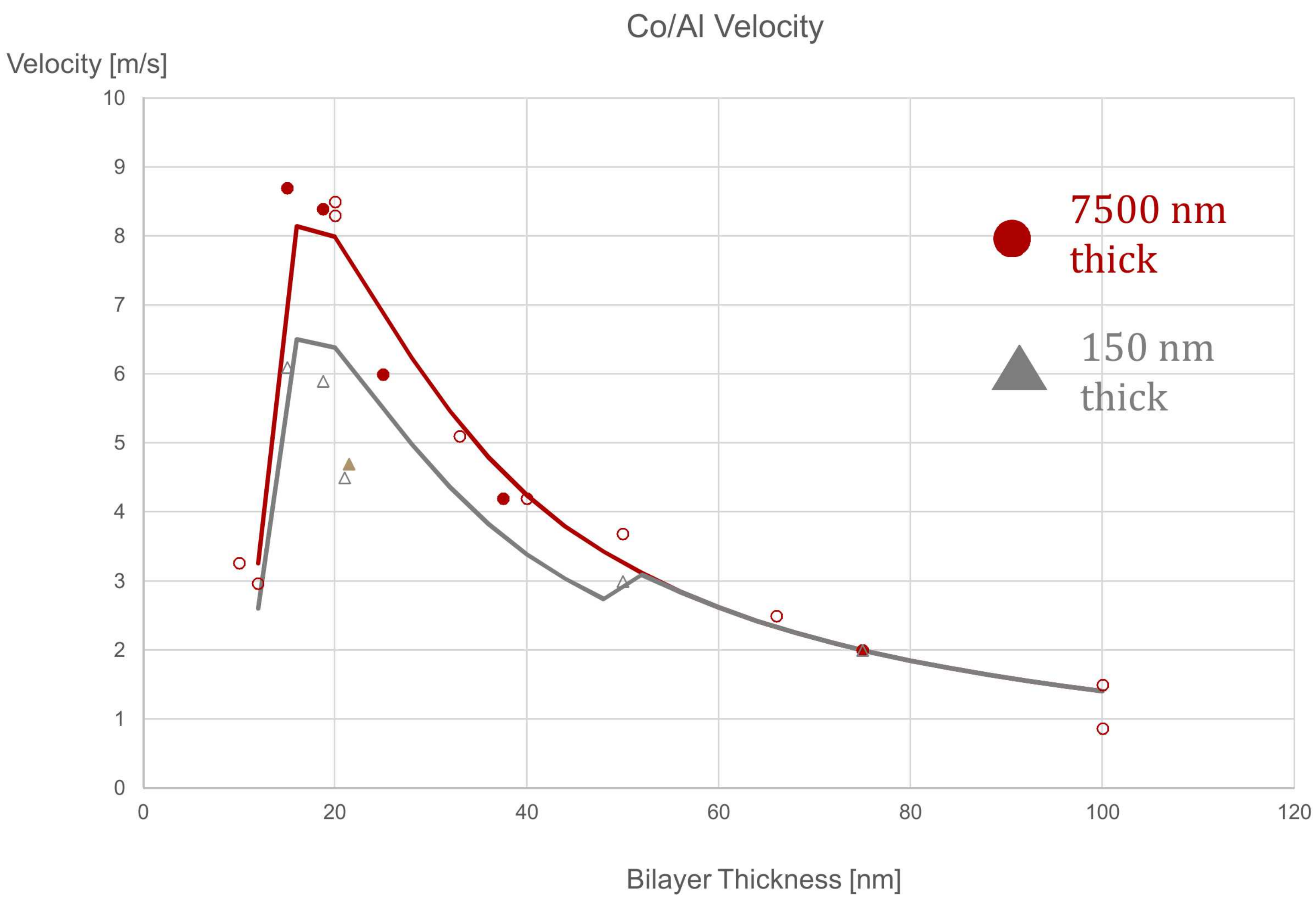
Flame temperature is determined based on the enthalpy/temperature diagram from the heat of reaction minus heat lost to radiation by:

$$Q_{rad}(T) = -\varepsilon \frac{2\sigma(T^4 - T_0^4)}{b_{Total\ Thickness}}$$





Matching to Experimental Data



Summary

We have populated the Mann model based on experimental data in order to fit values for activation energy and diffusion coefficient

This framework can be applied to the propagation of shock impacted samples to calculate changes in activation energy

Energy loss to the environment can be incorporated into the model based on its effects on flame temperature for studies involving self-propagation of electron transparent reactive nanolaminates