Significant back-flow of heat in multilayer nano-thin films subjected to femtosecond laser irradiation

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Introduction

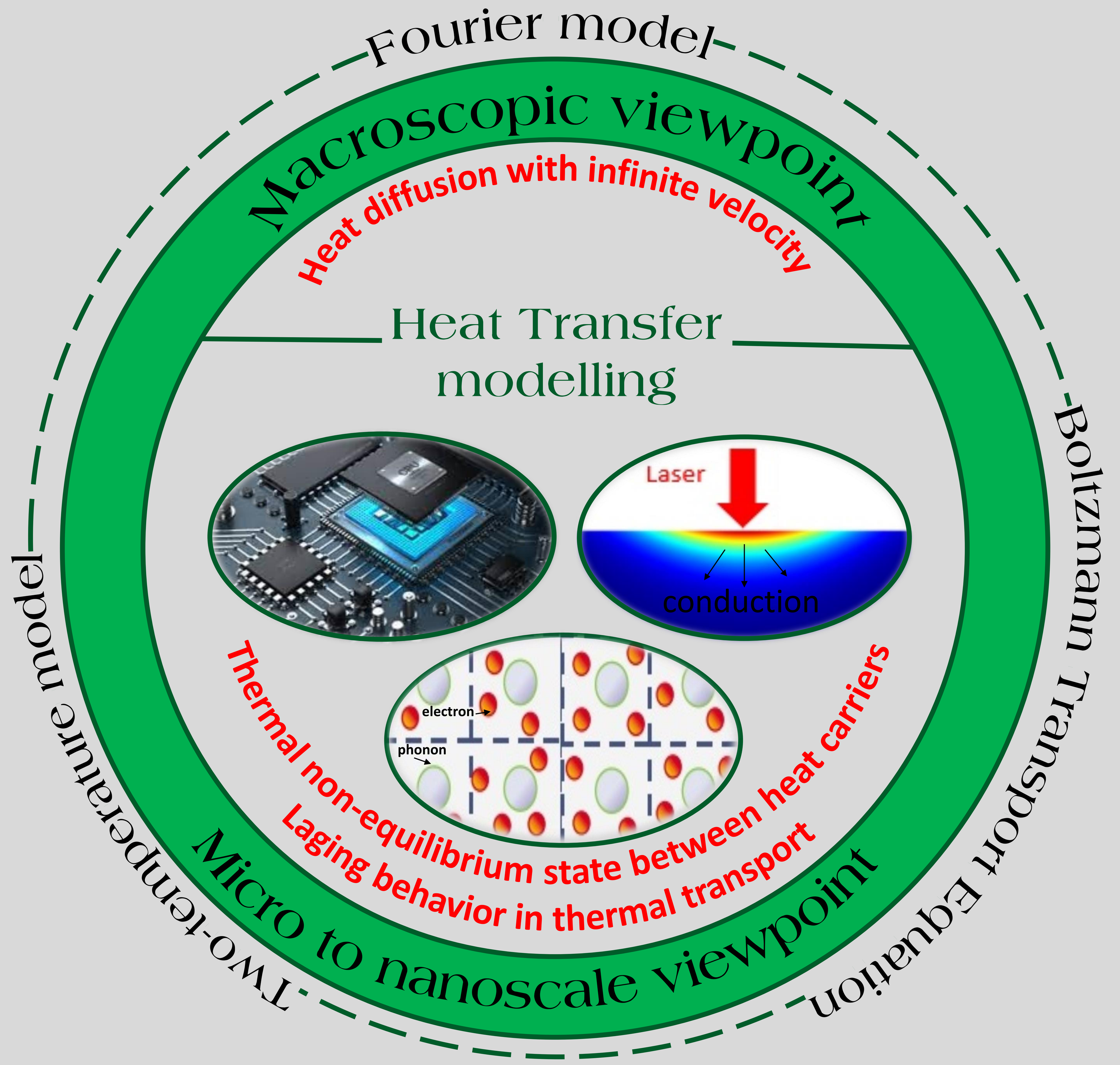
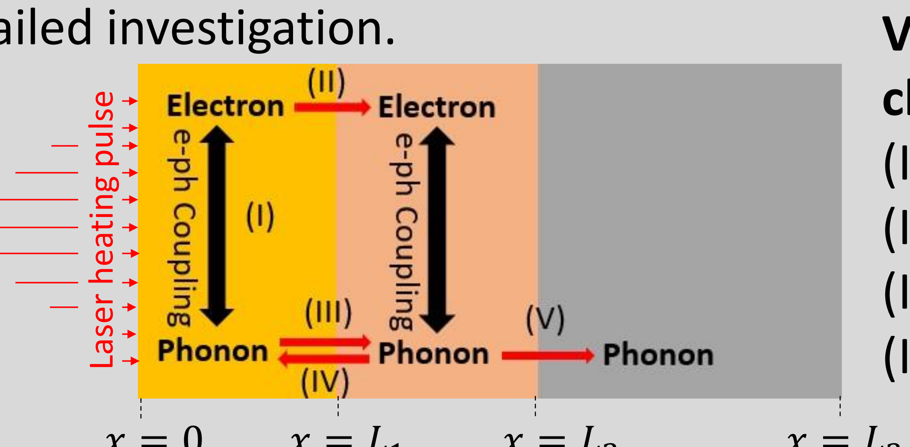


Fig. 1 Macro to nanoscale heat transfer modelling.

Problem & Methodology

To gain a better understanding of thermal response of multilayer nanosized structures under ultrafast laser irradiation, it is crucial to study the thermal transport mechanisms at play, particularly the interfacial electron and phonon transmissions that contribute to thermal conductance at the interface of different layers. Fig. 2 illustrates the significance of this research topic and the need for detailed investigation.



Various heat dissipation channels:

- (I) e-ph coupling.
- (II) Electron transmission.
- (III) Phonon transmission.
- (IV) Back-flow of thermal energy.

Fig. 2 Nanosized structure composed of Au top layer, Al interlayer and Si substrate, e: electron; ph: phonon.

- Boltzmann transport equation (BTE):

Electron energy equation: $C_e \frac{\partial e_e}{\partial t} + \vec{v}_e . \vec{\nabla} e_e = \frac{e_e^0 - e_e}{\tau_p} - G(T_e - T_p) + S(x,t)$ (1a)

Phonon energy equation: $C_p \frac{\partial e_p}{\partial t} + \vec{v}_p . \vec{\nabla} e_p = \frac{e_p^0 - e_p}{\tau_p} + G(T_e - T_p)$ (1b)

- Two-temperature model (TTM):

$$C_e \frac{\partial T_e}{\partial t} = k_e \nabla^2 T_e - G(T_e - T_p) + S(x,t) \quad (2a)$$

$$C_p \frac{\partial T_p}{\partial t} = k_p \nabla^2 T_p + G(T_e - T_p) \quad (2b)$$

- Gaussian femtosecond laser pulse function:

$$S(x,t) = \sqrt{\frac{\mu}{\pi}} \frac{(1-R)}{t_p(\delta_s + \delta_b)\left[1 - exp\left(\frac{-L}{\delta_s + \delta_b}\right)\right]} I_0 \, exp\left[-\frac{x}{(\delta_s + \delta_b)} - \mu\left(\frac{t - 2t_p}{t_p}\right)^2\right] \quad (3)$$

- Initial and boundary conditions:

$$T_e(x,0) = T_p(x,0) = T_0 = 300 \text{ K} \quad (4a)$$

$$\left.\frac{\partial T_{e,p}}{\partial x}\right|_{x=0,L_3} = 0, -k_{p,Au} \left.\frac{\partial T_{p,Au}}{\partial x}\right|_{x=L_1} = \left.\frac{T_{p,Au} - T_{p,Int}}{R_{pp,Au-Int.}}\right|_{x=L_1} \quad (4b)$$

(due to imperfect interface and different thermal properties)

In BTE, Eqs. (1a) and (1b), the energy density of electrons and phonons are related to the electron and phonon temperatures based on the following relationships,

$$e_e = \int_0^{T_e} C_e dT_e, C_e = \gamma_e T_e \rightarrow e_e = \int_0^{T_e} \gamma_e T_e d\,T_e \rightarrow e_e = 0.5 \gamma_e T_e^2 \quad (5a)$$

$$e_p = C_p T_p \quad (5b)$$

Results and discussion

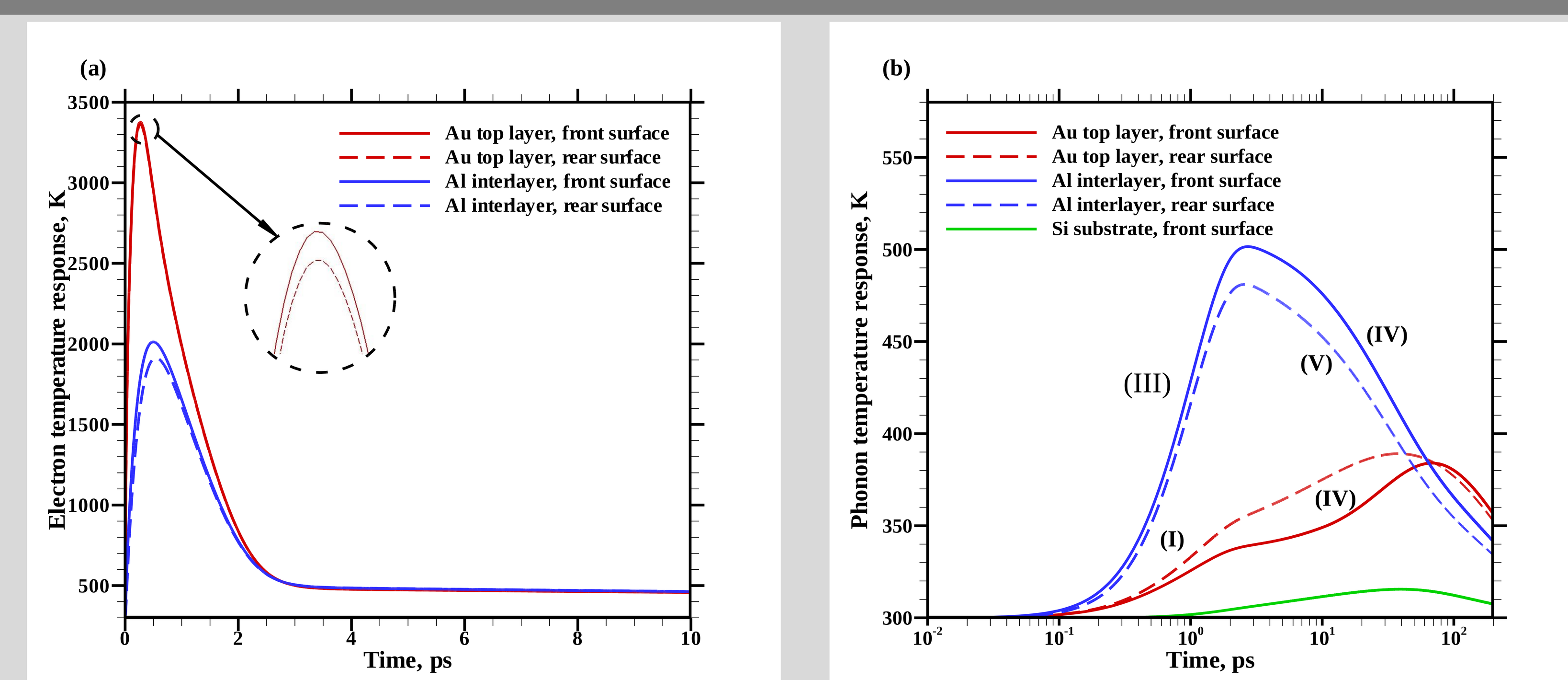


Fig. 3. Electron and phonon temperature response, 10-nm Au/10-nm Al/100-nm Si.

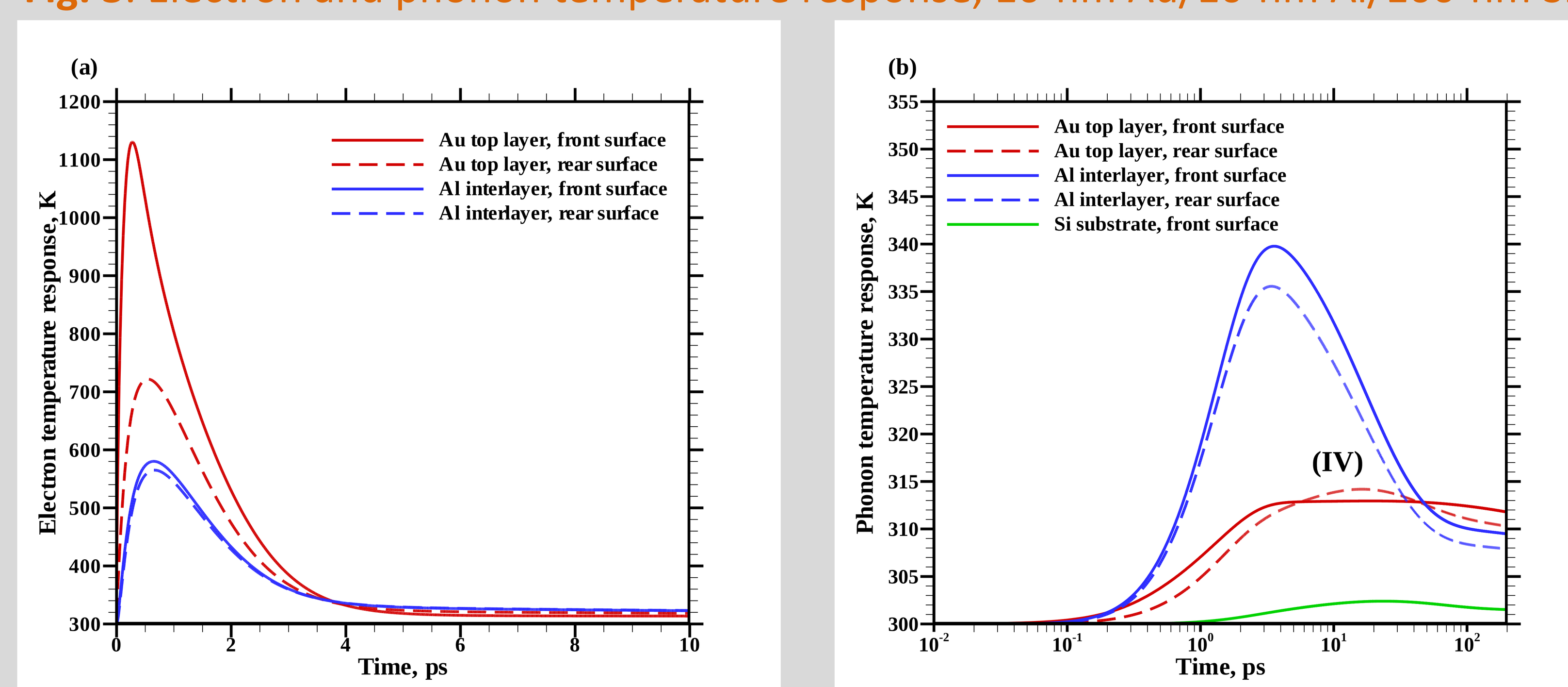


Fig. 4. Electron and phonon temperature response, 200-nm Au/10-nm Al/100-nm Si.

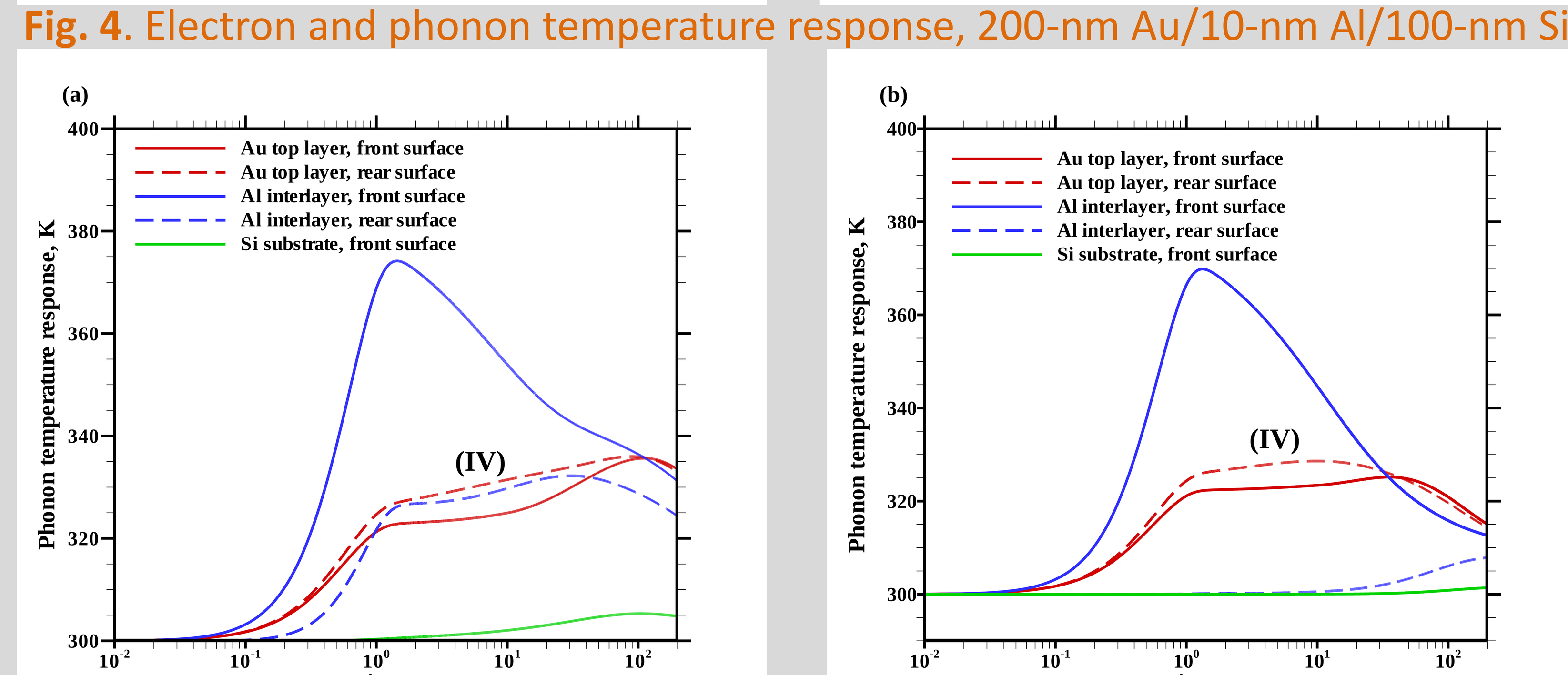


Fig. 5. Phonon temperature response, (a) 10-nm Au/50-nm Al/100-nm Si, (b) 10-nm Au/200-nm Al/100-nm Si.

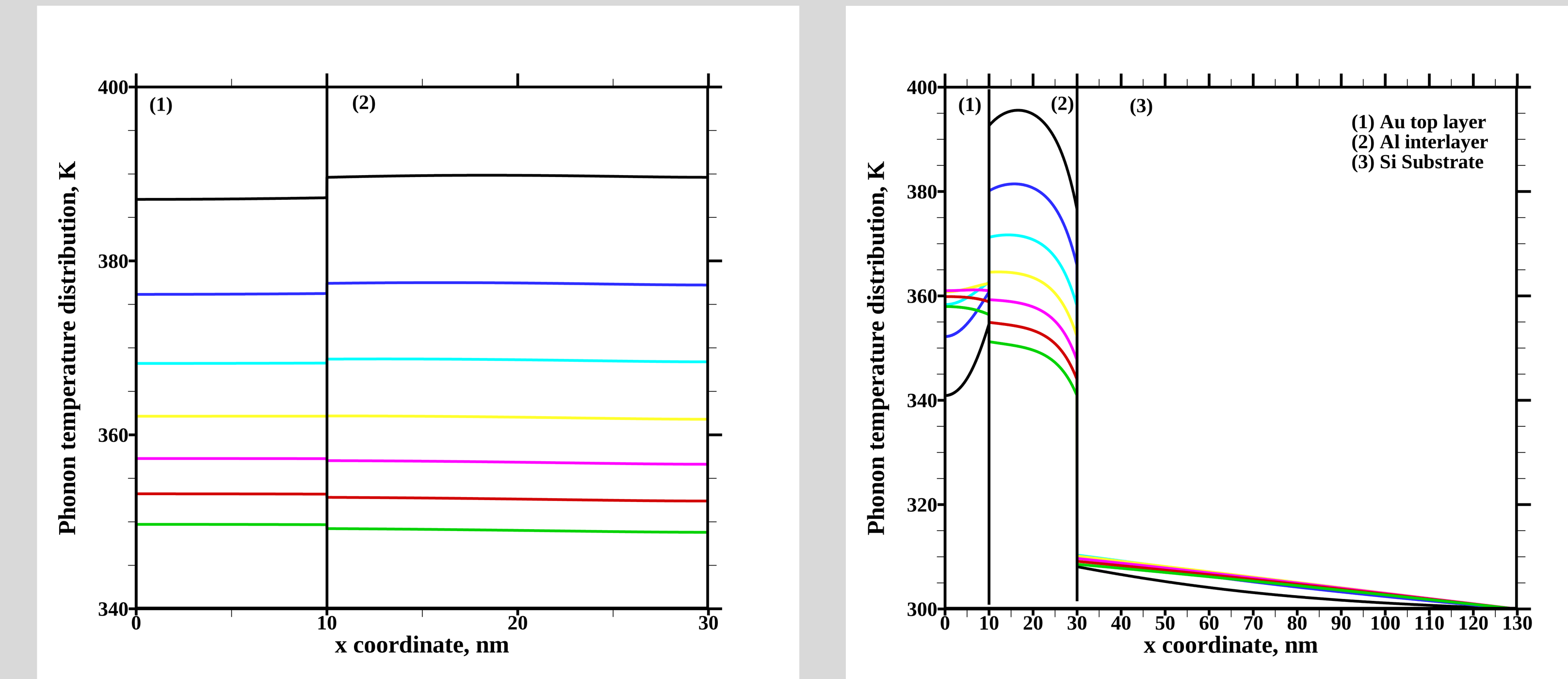


Fig. 6. Electron and phonon temperature distributions, 10-nm Au/20-nm Al/100-nm Si.

- The temperature response of electrons and phonons clearly illustrates the thermal non-equilibrium state, Figure 3.
- (I) Phonon temperature rise due to electron-phonon coupling, (III) phonon transmission at the interface of Au-Al, (IV) Back-flow of heat from hot Al lattice to Au top layer, (V) phonon transmission from Al interlayer to Si substrate, Figure 3.
- Thicker top layer film has a larger volume available to absorb thermal energy, which in turn can have a significant impact on back-flow of heat, Figure 4.
- An increase in interlayer thickness can impact the beck-flow of heat from interlayer to top layer, as the larger volume available for absorbing thermal energy plays a significant role, Figure 5.
- The electron and phonon temperature distributions show discontinuity at the interface of different layers, because there is thermal resistance between materials with different vibrational properties, Figure 6.

Conclusions

- The addition of an interlayer with a high e-ph coupling factor can enhance the cooling of electrons, thereby mitigating the thermal damage in Au thin film.
- The insertion of an interlayer can create distinct heat dissipation channels at the interface of Au, Al and Si layers, involving both electrons and phonons.
- The transmission of phonons at the interface of Au and Al can lead to the back-flow of heat, which in turn can rise the phonon temperature of Au layer.
- The phenomenon of heat back-flow can be harnessed as a novel method for gently heating materials supported on a metal substrate, offering a unique approach to thermal processing.

Acknowledgement

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