Two-temperature time-fractional model for electron-phonon coupled interfacial thermal transport

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Introduction

- At nanoscale, the heat carriers e.g., electrons and phonons play a vital role in heat transfer mechanism, Figure 1.

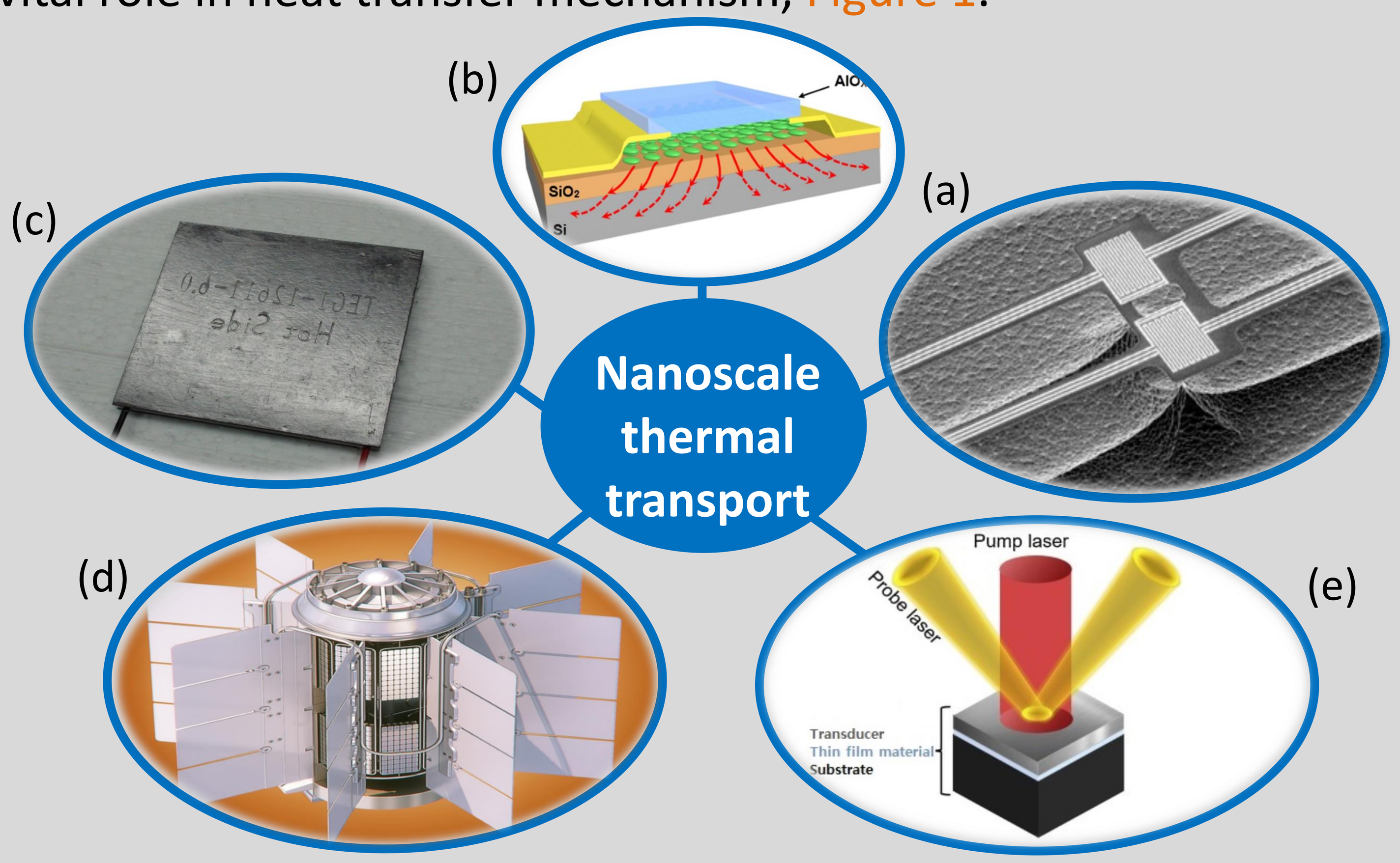

Figure 1 Thermal transport in nano-electronic devices and multilayered samples.

a) Better understanding of thermal processes at nanoscale can lead to more effective design of nanoscale devices.
b) The better cooling of nano-electronic devices can improve their lifetime. Nano-sandwiching can prevent overheating in nano-electronic devices.
c) The thermoelectric materials have been used for effective cooling of nanoscale devices.
d) Such materials are also utilized in radioisotope thermoelectric generator to convert waste heat into electricity to power space probes.
e) The pump-probe laser based technique can be effectively used to determine the unknown thermal properties of different materials, including the thermoelectric materials.

Problem

The complexity of 2T-BTE model and high computational cost involved (Wang et al. 2016) would lead us to the use of fractional calculus approach to improve the conventional 2T model with less computational cost and the high accuracy comparable to the 2T-BTE simulations. The schematic of multilayered films and imperfect interface are depicted in Figure 2.

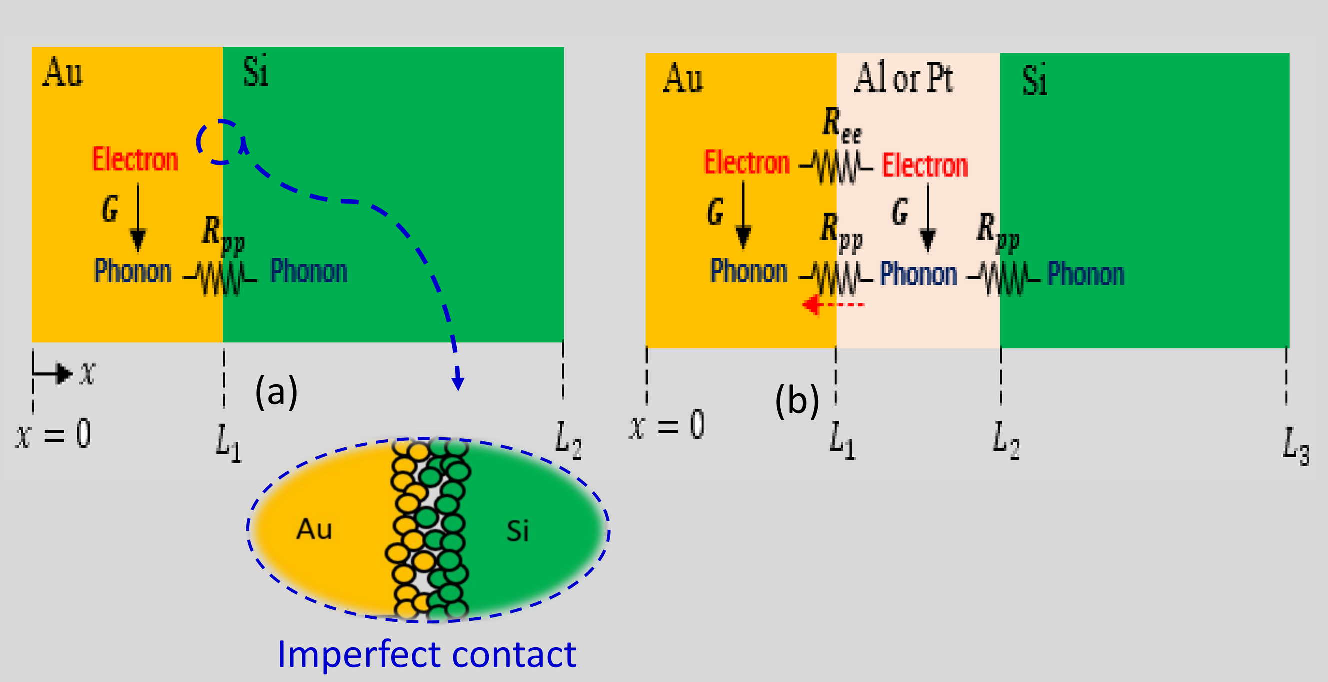

Figure 2 (a) Au 20 nm/Si 100 nm film without interlayer, and (b) Au/Si film with an interlayer Al or Pt 20 nm.

- Two-temperature time-fractional (2T-TF) model:

Electron energy equation: $C_e \frac{\partial^\beta T_e}{\partial t^\beta} = k_e \tau_e^{1-\beta}\frac{\partial^2 T_e}{\partial x^2} - G(T_e - T_p) + S(x,t)$ (1a)

Phonon energy equation: $C_p \frac{\partial T_p}{\partial t} = k_p \frac{\partial^2 T_p}{\partial x^2} + G(T_e - T_p)$ (1b)

- Gaussian femtosecond laser pulse function:

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

- Initial and boundary conditions:

$T_e(x,0)=T_p(x,0)=T_0=300\ \mathrm{K}$ (3a)

$$\left.\frac{\partial T_{e,p}}{\partial x}\right|_{x=0,L_2}=0, -k_{p,Au}\left.\frac{\partial T_{p,Au}}{\partial x}\right|_{x=L_1} = \left.\frac{T_{p,Au}-T_{p,Si}}{R_{pp,AuSi}}\right|_{x=L_1}$$ (due to imperfect interface and different thermal properties) (3b)

Methodology

- The discrete form of phonon energy equation:

$$T_{p,i}^n = \left[1 - \frac{2k_p\Delta t}{\Delta x^2 C_p} - \frac{G\Delta t}{C_p}\right]T_{p,i}^{n-1} + \left[\frac{k_p\ \Delta t}{\Delta x^2 C_p}\right](T_{p,i+1}^{n-1}+T_{p,i-1}^{n-1}) + \left[\frac{G\Delta t}{C_p}\right]T_{e,i}^{n-1} \quad (4)$$

- The discrete form of electron energy equation:

$$\left[\frac{k_e\tau_e^{1-\beta}}{\Delta x^2}\right]T_{e,i-1}^n - \left[\frac{2k_e\tau_e^{1-\beta}}{\Delta x^2}+C_e\sigma_\beta+G\right]T_{e,i}^n + \left[\frac{k_e\tau_e^{1-\beta}}{\Delta x^2}\right]T_{e,i+1}^n = -C_e\sigma_\beta T_{e,i}^{n-1} + C_e\sigma_\beta\sum_{j=2}^{n}\omega_j^\beta\left(T_{e,i}^{n-j+1}-T_{e,i}^{n-j}\right) - GT_{p,i}^n - S(i,n) \quad (5)$$

where σ_β and ω_j^β are defined as follow (Mozafarifard and Toghraie 2020),

$$\sigma_\beta = \frac{1}{(1-\beta)\Delta t^\beta \Gamma(1-\beta)}, \omega_j^\beta = [j^{1-\beta}-(j-1)^{1-\beta}] \quad (6)$$

To guarantee the stability of numerical solution of Eqs. (4) and (5), the mesh steps are considered as $\Delta t = 0.0004$ ps and $\Delta x = 0.5$ nm, satisfying the convergence condition as $[1 - 2k_p\Delta t/\Delta x^2 C_p] \geq 0$.

Results and discussion

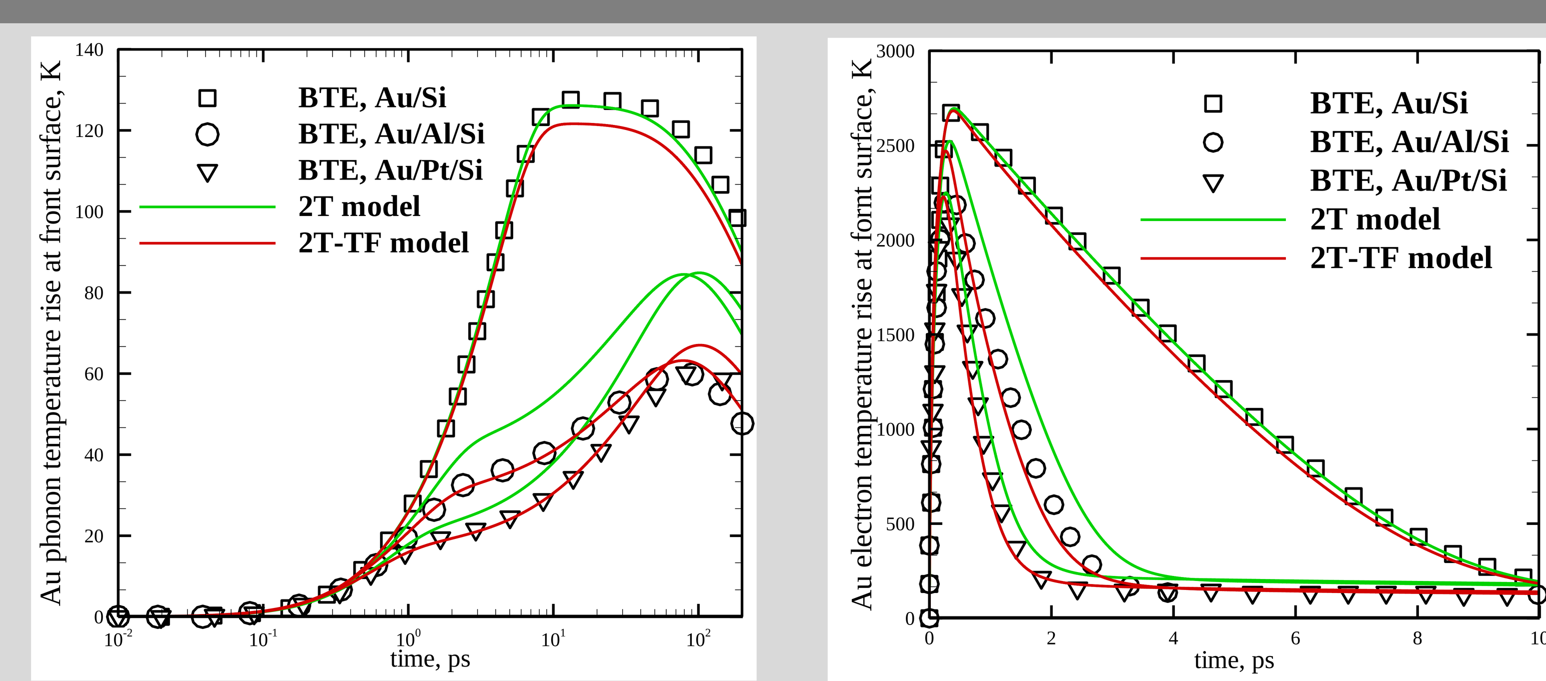

Figure 3 Electron and phonon temperatures, for Au/Si sample: $\beta = 0.99$, for Au/Si with an interlayer: $\beta = 0.9$.

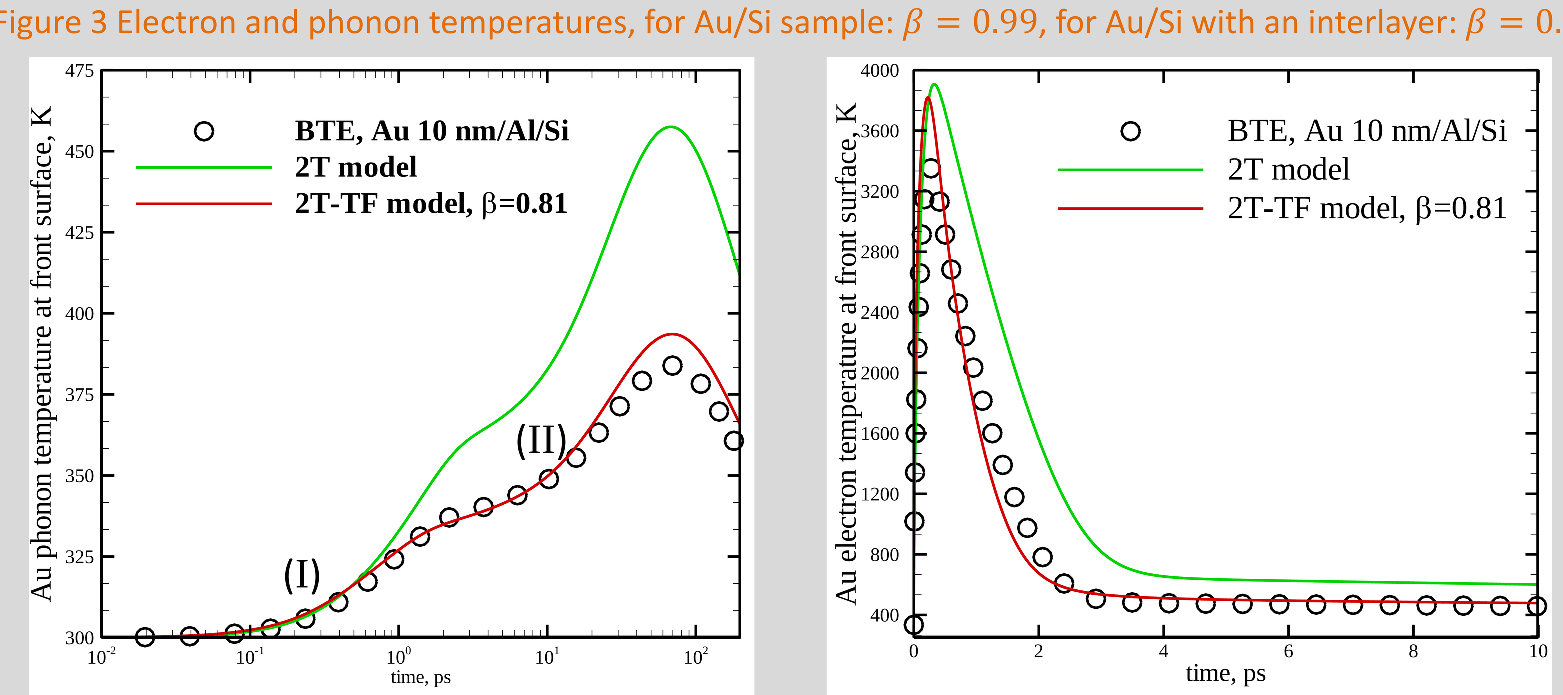

Figure 4 The effect of thickness on heat transfer mechanism of Au/Al/Si film.

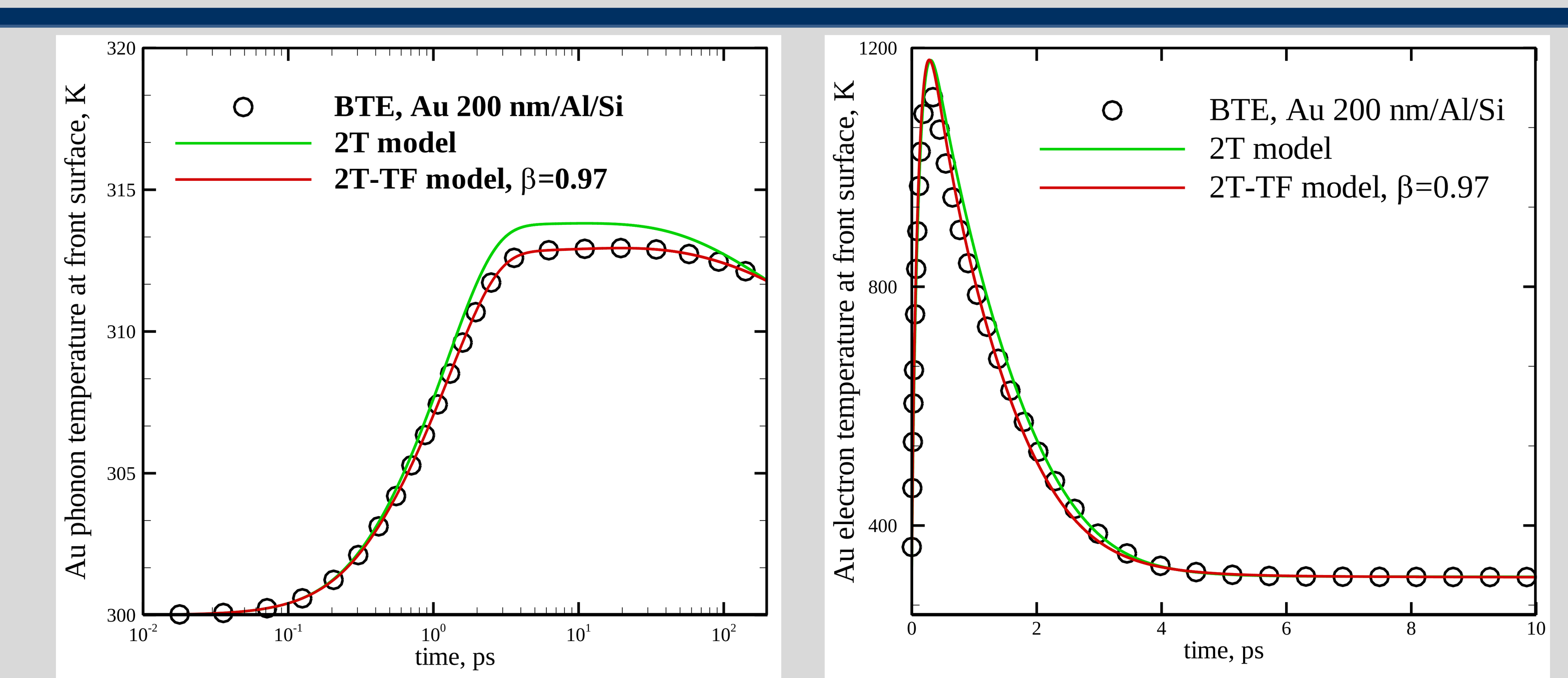

Figure 5 The effect of thickness on heat transfer mechanism of Au/Al/Si film.

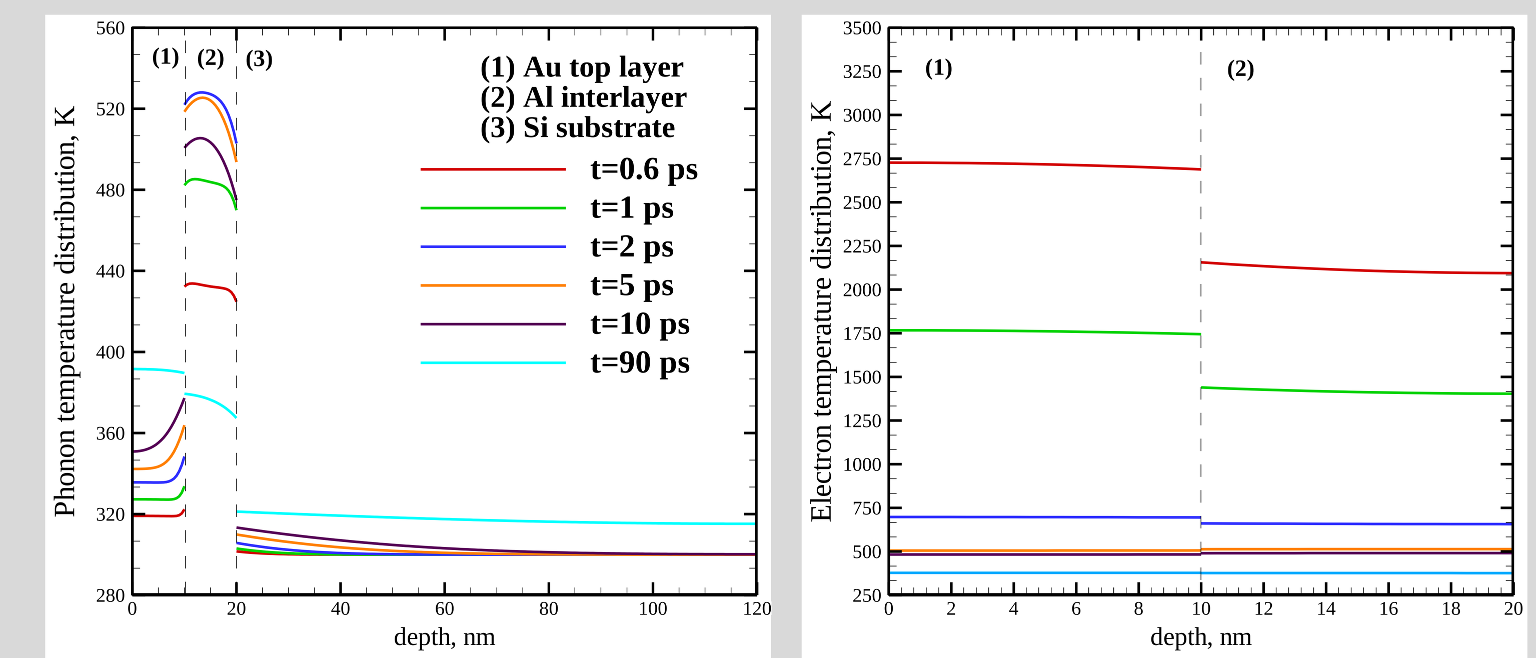

Figure 6 Electron and phonon temperature distributions through the sample, 2T-TF model with $\beta = 0.81$.

- Ballistic effects are negligible for Au/Si film, and thermal transport is diffusive, Figure 3.
- (I) Heat transport from electrons to the lattice, (II) Back-flow of thermal energy from the interlayer to the Au lattice. The non-Fourier effects are significant for Au top layer with small thickness, Figure 4.
- For greater thickness of Au top layer, the diffusive-like behaviors can be seen in thermal transport of Au/Al/Si film, Figure 5.
- The discontinuity in temperature distribution of multilayered film is due to the different thermal properties, which creates the heat dissipation channels at the interface of various layers, Figure 6.

Conclusions

- Inserting an interlayer with high electron-phonon coupling factor can lead to more rapid electron and phonon cooling in Au top layer.
- The back-flow of thermal energy from interlayer to the Au top layer would increase the lattice temperature of Au layer.
- The order of fractional derivative can be a measure of intensity of the ballistic effects or non-diffusive behaviors.
- The 2T-TF model can provide accurate description of thermal transport of multilayered films with less computational cost and complexity compared to 2T-BTE model, so it can be used in TDTR technique to accurately calculate the thermophysical properties of materials.

Acknowledgement

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References

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