Interfacial Electron and Phonon Scattering Processes in High-Powered Nanoscale Applications

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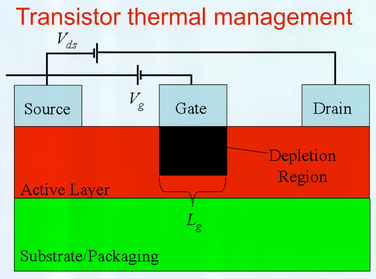
Problem

Electron-phonon (ep) scattering is a limiting form of thermal resistance in several nano-applications

Transistor thermal management

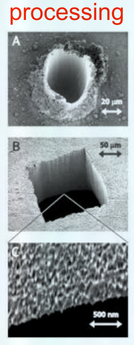


$$E \propto \sqrt{\frac{V}{L_g}}$$

Increase V
Decrease L_g

Large E means large ep scattering

Thin film laser processing



Short pulses induce large ep nonequilbrium

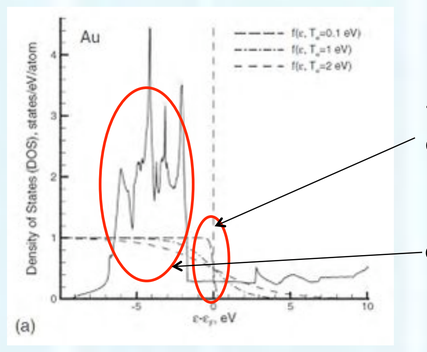
Thermoelectric design

$$Z = \frac{S^2\sigma}{k}$$

ep scattering at interfaces will affect k

Study electron/interface scattering processes after short pulsed laser heating

- Substrate/interface influence during electron-phonon coupling
- Ballistic diffusive approximation to Boltzmann Transport Equation (BTE)
- d-band electron excitation influence on thermal properties
- Influence of d-band excitation on ballistic transport



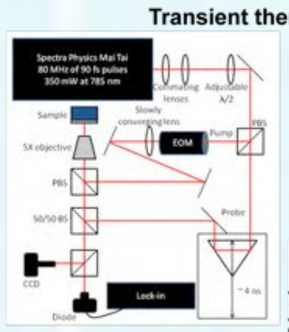
Typical transport analyses – free electrons (s/p conduction bands)

Large fluxes/temperatures excite d-band electrons – how do these affect transport?

Approach

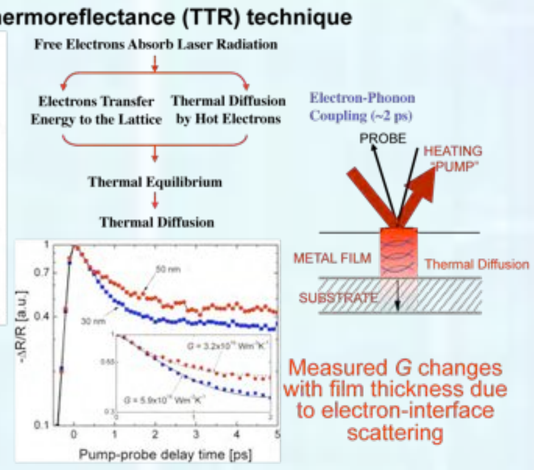
Transient thermoreflectance (TTR) technique

Transient thermoreflectance (TTR) technique



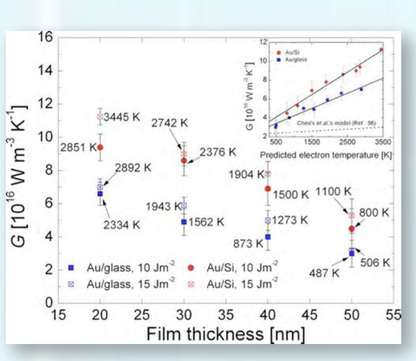
TTR data fit to two-temperature model

Electron-phonon coupling factor = G

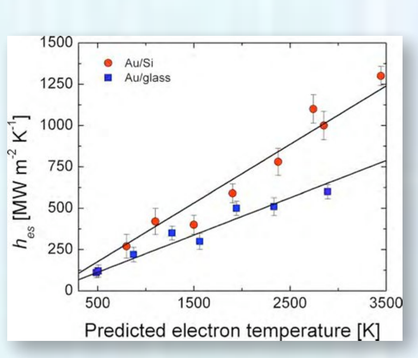


Measured G changes with film thickness due to electron-interface scattering

Results



Film thickness and substrate dependence suggests ballistic electron-interface scattering.



Use three-temperature model (3TM) to determine h_{es}

Hopkins *et al.*, Journal of Applied Physics, **105**, 023710 (2009)

Results (cont.)

Ballistic diffusive approximation (BDA) to the BTE for electron transport

BTE for electrons

$$\frac{\partial f}{\partial t} + v_z\frac{\partial f}{\partial z} + \frac{F_z}{m}\frac{\partial f}{\partial v_z} = \left(\frac{\partial f}{\partial t}\right)_c$$

BTE: thin film limit

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_c$$

Equation of Electron Energy Transfer (EEET)

$$\frac{\partial U_\varepsilon(t)}{\partial t} = \left(\frac{\partial U_\varepsilon(t)}{\partial t}\right)_c \qquad U_\varepsilon = \varepsilon D(\varepsilon) f(1-f)$$

BDA to the BTE - no electron/substrate energy loss

$$\frac{\partial U_\varepsilon}{\partial t} = \frac{\partial}{\partial t}\left(U_{\varepsilon,b}(t) + U_{\varepsilon,m}(t)\right) = -\frac{U_{\varepsilon,b} - U_{\varepsilon,m}}{\tau_{ee}} - \frac{U_{\varepsilon,m} - U_{\varepsilon,0}}{\tau_{ep}}$$

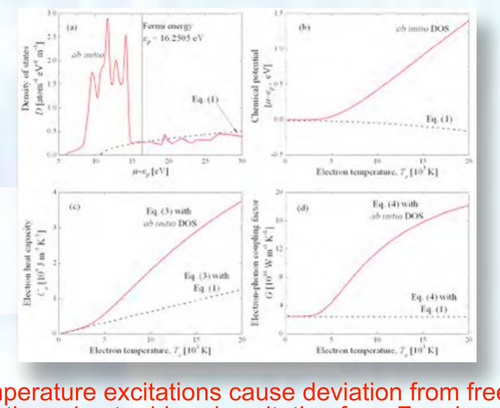
Chen, Journal of Heat Transfer, **120**, 320-328 (2002)

BDA to the BTE - electron/substrate energy loss

$$\frac{\partial U_\varepsilon}{\partial t} = \frac{\partial}{\partial t}\left(U_{\varepsilon,bi} + U_{\varepsilon,m}\right) = -\frac{U_{\varepsilon,bi}}{\tau_{ei}} - \frac{U_{\varepsilon,0}(T_e) - U_{\varepsilon,0}(T_p)}{\tau_{ep}}$$

Hopkins and Norris, Journal of Heat Transfer, **131**, 022402 (2009)

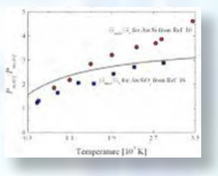
Follow Lin, *et al.* (PRB, 77, 075133 (2008)) with Au.pz-d-rrkjus.UPF pseudopotential from the http://www.quantum-espresso.org distribution



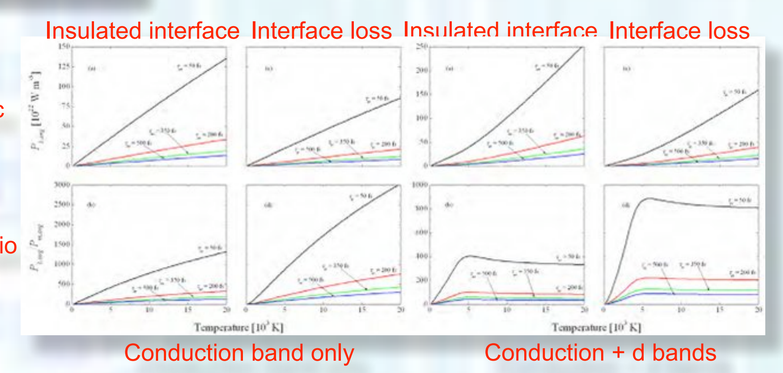
High-temperature excitations cause deviation from free electron predictions due to d-band excitation from Fermi smearing

Hopkins and Stewart, to appear in the Journal of Applied Physics

Power density in ballistic and diffusive electron regimes



Ballistic diffusive (B/D) solution to BTE matches experimental data well when accounting for electron-interface scattering



Conduction band only

Conduction + d bands

Significance

- Pump-probe TTR measurements show enhancement of electron system energy loss due to the presence of an interface in thin Au films.
- Electron-interface scattering is substrate dependent, indicating that it is a thermal process.
- Model electron-interface scattering with BDA to the BTE to separate electron-phonon coupling from electron-interface processes — excellent agreement with experimental evidence in "low" temperature limit.
- "High" temperatures can induce sub-conduction band excitations, drastically affecting thermal properties.
- Interface scattering can enhance thermal removal from heated region if thermal processes are ballistic before interface scattering.

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