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Research Paper

Thermal transport in thin dielectric films with minute size aluminum dot in relation to microelectronics

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HIGHLIGHTS

- Equivalent equilibrium temperature increases in close region of aluminum dot.
- Low temperature edges of film act like phonon sink lowering phonon intensity in close region to edges.
- Temporal variation of equivalent equilibrium temperature does not follow temperature distribution at aluminum dot edge.
- Emitted phonons undergo scattering in close region of aluminum dot modifying temporal response of temperature.

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ABSTRACT

Thermal energy transfer across the thin silicon and diamond films with the presence of aluminum minute size dot is studied. The thin films are thermally disturbed by the aluminum dot edges at which the time is exponentially increasing temperature profile was introduced. Transient and frequency dependent Boltzmann equation is incorporated to formulate the phonon transport across the film. A numerical solution incorporating the discrete ordinate method is adopted to compute the phonon intensity distribution. The equivalent equilibrium temperature is introduced to quantify the phonon intensity distribution, in terms of temperature variation, in the film. It is found that equivalent equilibrium temperature decays sharply in the close region of the aluminum dot because of scattering of emitted phonons from the aluminum dot edge. Temporal variation of equivalent equilibrium temperature does not follow exactly temperature rise at the aluminum dot edge because of scattering of phonons in the film.

1. Introduction

Thermal management of thin films in electronic devices is critical for maintaining the high performance of processing [1]. Heat transfer across thin films is governed by the phonon transport and depending on the film size and thermal disturbance across the film [2], the ballistic phonons contribute significantly to the energy transport within the film [3]. As the thickness of the film becomes comparable to the phonon mean free path, non-equilibrium energy transport governs within the film. The classical approaches, such as Cattaneo and Fourier heating models, to the solution of the problem, fail to predict correct energy transport characteristics within the film [4,5]. However, the use of the Boltzmann equation covers the non-equilibrium characteristics of energy transport and provides a solution to the heating problem [6]. Since the phonons are the energy carriers having various frequencies, like photons, the transport process can mimic the radiative characteristics of the film [6]. Consequently, introducing the phonon radiative transport in the film gives rise to accurate prediction of the thermal energy transport inside the film when subjected to the thermal disturbance. To quantify the phonon intensity distribution in terms of the thermodynamic properties, such as temperature, an equivalent equilibrium temperature is introduced in the thin film [7]. This is because of the fact that the local thermodynamic equilibrium condition is not satisfied in terms of a thermal equilibrium state; therefore, the equivalent equilibrium temperature is considered for the phonons when the intensities are redistributed adiabatically to an equilibrium state. Therefore, it represents the average energy of all phonons around a local point and it is equivalent to the equilibrium temperature of phonons when they redistribute adiabatically to an equilibrium state [7]. In the case of presence of the minute size metallic quantum dot inside the film, thermal disturbance gives rise to

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Nomenclature

C_k	frequency dependent volumetric specific heat capacity of the dielectric material
D	density of state
f_k	frequency dependent probability distribution function in phase space
f_k^0	equilibrium probability distribution function in phase space
$\hbar$	reduced Planck's constant
I_k	frequency dependent phonon intensity
I_k^{++}	frequency dependent phonon intensity in the first quadrant
I_k^{-+}	frequency dependent phonon intensity in the second quadrant
I_k^{+-}	frequency dependent phonon intensity in the third quadrant
I_k^{--}	frequency dependent phonon intensity in the fourth quadrant
I_k^0	frequency dependent equilibrium phonon intensity
k	wavenumber
$L_{Q,Dot}$	dimension of the quantum dot
L_x	thickness of the silicon film
L_z	width of the silicon film
q''_x	heat flux in the x-direction
q''_z	heat flux in the z-direction
t	time
T	equivalent equilibrium phonon temperature
u	internal energy density of phonon
v_k	frequency dependent group velocity of phonons
x	Cartesian coordinate x-direction
z	Cartesian coordinate z-direction
Δx	grid spacing in the x-direction
Δz	grid spacing in the z-direction

Greek symbols

Λ_k	frequency dependent phonon mean-free-path
θ	polar angle
ϕ	azimuthal angle
τ_k	frequency dependent relaxation time
ω	frequency

Subscript

A	sub-domain A
B	sub-domain B
C	sub-domain C
D	sub-domain D
LA	longitudinal acoustic
LO	longitudinal optical
TA	transverse acoustic
TO	transverse optical
x	x-axis
z	z-axis

complicated energy transfer characteristics inside the film. The location of the metallic dot to the thermal disturbing sites becomes critical for the phonon intensity distribution inside the film [8]. Consequently, investigation of the thermal energy transport within the thin dielectric film with the presence of the minute size metallic dot becomes essential.

The structural/property changes in the thin film, such as metallic dots in dielectric film, or presence of film pairs with different thermo-physical properties modify the phonon transport characteristics in the film when subjected to a thermal disturbance. In this case, the cross-plane transport takes place across the structural/property changes in the film [9]. For example, the cross-plane heat conduction in nanoporous silicon thin films was studied by Hua and Cao [9]. They demonstrated that the effective thermal conductivity varied not only with the porosity but also with the film thickness and pore radius. The smaller the film thickness or the pore radius, the smaller was the effective thermal conductivity for a given porosity. In addition, an analytical study of phonon transport in periodic bulk nanoporous structures was carried out by Hao et al. [10]. They incorporated assumption of diffusive phonon scattering by pore edges to predict the lattice thermal conductivity via modifying the bulk phonon mean free paths with the characteristic length of the nanoporous structure. In perfect films also fall into this category and phonon transport characteristics changes across the film. One of the applications was introduced for imperfect graphene by Wang et al. incorporating the first-principle solution towards predicting the thermal and infrared spectra [11]. The findings revealed that the peaks of phonon density of states occurred at about 40 and 45.5 THz in the perfect graphene (G) and they were shifted to 40.5 and 46 THz in the imperfect graphene (G-D), respectively. The presence of quantum dots in thin films gices rise to phonon confinement in the film. This issue was addressed in nanostructured thin films by Pejova [14]. The findings revealed that relaxation time characterizing the phonon decay processes in as-deposited samples was found to be approximately 0.38 ps, while upon post-deposition annealing at 200 °C, it increased to about 0.50 ps. Both of these values were, however, significantly smaller than those characteristic for a macrocrystalline ZnSe sample. The film size [12] and film shape, such as curvature [13], influence the phonon transport charactecs and film properties, such as thermal conductivity. The lattice dynamics analysis of thermal conductivity in silicon nanoscale film was carried out by Wang and Li [12]. They indicated that there existed the obvious size effect on the thermal conductivity when the film thickness reduced to nanoscale or microscale, and the feasibility of the molecular dynamics method was a particularly good alternative method to investigate the physical characteristics of the nano-size film when the direct measurement was difficult to make. Phonon transport across the nano-scale curved thin film was investigated by Mansoor and Yilbas [13]. They demonstrated that reducing film arc angle increased the film curvature; in which case, phonon intensity decay became sharp in the close region of the high temperature edge. Temperature distribution demonstrated non-symmetric behavior along the radial direction, which was more pronounced in the near region of the high temperature edge. However, in thin films pairs constituting different film properties with presence of structural discontinues, such as vacuum gaps, ballistic phopnons plays a major role for phonon transport across the planes. Such application was presented by Yilbas and Haider [15] through considering ballistic phonon and thermal radiation transport across a minute vacuum gap in between the aluminum and the silicon thin films when subjected to the laser irradiation pulse. It was shown that thermal separation of electron and lattice sub-systems in the aluminum film took place and electron temperature remained high in the aluminum film while equivalent equilibrium temperature for phonons decayed sharply