407.Accession number:12988109
Title:Pressure dependency of thermal boundary conductance of carbon nanotube/silicon interface: a molecular dynamics study
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Source title:Journal of Applied Physics
Abbreviated source title:J. Appl. Phys. (USA)
Volume:112
Issue:5
Publication date:1 Sept. 2012
Pages:053501 (5 pp.)
Language:English
ISSN:0021-8979
CODEN:JAPIAU
Document type:Journal article (JA)
Publisher:American Institute of Physics
Country of publication:USA
Material Identity Number:DK28-2012-027
Abstract:Thermal boundary conductance (TBC) of open carbon nanotube (CNT) and crystal silicon was investigated by the method of molecular dynamics (MD) simulation. Van der Waals interaction was used to form the interface between the vertically mounted CNT and the silicon surface. The interfacial TBC was extracted from the thermal relaxation between CNT and Si with different initial temperatures. An enhancement of TBC was spotted with the increase of the external pressure. At the interfacial region, the phonon densities of states of CNT and Si were altered by the external pressure, especially at the frequency between 2 THz and 15 THz, which could be associated with the enhancement of TBC.
Number of references:23
Inspec controlled terms:carbon nanotubes - elemental semiconductors - heat conduction - interface phonons - molecular dynamics method - silicon - thermal conductivity
Uncontrolled terms:external pressure dependency - thermal boundary conductance - carbon nanotube-silicon interface - open carbon nanotubes - molecular dynamics simulation - Van der Waals interaction - VdW interaction - vertically mounted CNT - silicon surface - interfacial TBC - thermal relaxation - interfacial region - phonon densities of states - frequency 2 THz to 15 THz - C-Si
Inspec classification codes:A6670 Nonelectronic thermal conduction and heat-pulse propagation in nonmetallic solids - A6830 Dynamics of solid surfaces and interface vibrations
Numerical data indexing:frequency 2.0E+12 1.5E+13 Hz
Chemical indexing:C-Si/int Si/int C/int Si/el C/el
Treatment:Theoretical or Mathematical (THR)
Discipline:Physics (A)
DOI:10.1063/1.4749798
Database:Inspec