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Using cube models to understand trends in thermal accommodation coefficients at high surface temperatures

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ABSTRACT

Knowledge of the thermal accommodation coefficient (TAC) at high surface temperatures is critical in many applications, including sizing of aerosolized nanoparticles through time-resolved laser-induced incandescence (TiRe-LII). Unfortunately, an understanding of the fundamental physics that underlies this parameter is elusive. To this end, we carry out a comparative analysis of the hard, soft, and washboard cube model predictions and contrast these with molecular dynamics results on helium scattering from high temperature solid and molten silicon surfaces. This treatment elucidates the key physics underlying trends in the TAC with respect to the gas molecule to surface atom mass ratio and the gas-surface temperature ratio at surface temperatures between 1500 and 3000 K.

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1. Introduction

There are many applications in science and engineering in which it is important to characterize the energy transfer between a surface and free-molecular gas. For instance, this knowledge is needed in order to: model how carbon nanotubes (CNTs) perform as gas sensors [1,2]; develop film coatings to enhance heat transfer [3]; analyze the storage of hydrogen in carbon nanotubes [4–6]; and understand the growth mechanisms of gas-phase nanoparticle synthesis [7–9]. Free-molecular heat conduction is also central to time-resolved laser-induced incandescence (TiRe-LII) [10–12], a diagnostic used to infer the size distributions of aerosolized nanoparticles. In this technique, nanoparticles within a sample volume of aerosol are heated using a laser pulse to incandescent temperatures. The spectral incandescence decay is then measured, usually at multiple wavelengths, as the nanoparticles equilibrate with the bath gas. A spectroscopic model is used to derive an effective temperature from the spectral intensity measurements, and, since the nanoparticle cooling rate depends on the surface-to-volume ratio, the nanoparticle size distribution can be inferred from the temperature decay using a heat transfer model.

Free-molecular conduction depends on the incident number flux of gas molecules as well as the average energy transfer when gas molecules scatter from the surface. This energy transfer is quantified by the thermal accommodation coefficient (TAC),

$$\alpha = \frac{\langle E_o - E_i \rangle}{\langle E_o - E_i \rangle_{max}} \tag{1}$$

where $\langle \cdot \rangle$ denotes an average, and E_i and E_o are the incident and scattering energy of the gas molecule respectively. The denominator represents the maximum energy transfer allowed by the Second Law of Thermodynamics, which would occur if the gas molecules were to equilibrate with the surface. Saxena and Joshi [13] provide an extensive summary of experimentally-derived TACs reported prior to 1980. These and more recent studies highlight how the TAC depends on key parameters [14,15], including the: mass ratio, $\mu = m_g/m_s$, where m_g is the gas molecular mass and m_s is the surface atomic mass [15–18]; temperature ratio, $\tau = T_g/T_s$, where T_g and T_s are the gas and surface temperatures respectively [15,16,19]; surface roughness [14,15,20]; and lattice frequency. Molecular dynamics (MD) simulations have also elucidated how the TAC varies with the mass ratio [21–24], surface temperature [21,25–27], and potential well depth [6,25,28], mostly for surfaces near room temperature. Fig. 1a shows a sample of experimentally-[29–31] and MD-derived [21,26] TACs as a function of T_s for mass ratios close to $\mu = 0.2$ (specifically Pt-Ar, Au-Ar, and Si-He). The figure shows that the molecular dynamics simulations capture the main experimentally-observed trends.

Unfortunately, few scattering experiments and MD simulations, including those shown in Fig. 1a, are carried out at high surface temperatures (>1500 K [13,19]). In this regime, $T_s \gg T_g$, so the scattered gas molecular trajectories are strongly influenced by the thermal motion of the surface atoms and $k_B T_s$ is much larger than

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Nomenclature

Nomenclature and abbreviations

a	morse potential parameter [nm]
A	Baule equation constant
D	gas-surface potential well depth [meV]
E_o	reflected or outgoing kinetic energy [J]
E_i	incident kinetic energy [J]
f_k	surface atom (or cube) frequency [Hz]
HC	abbreviation for hard cube model
$K(\boldsymbol{v}_1,\boldsymbol{v}_2)$	gas scattering kernel
k_B	Boltzmann constant, 1.3806×10^{-23} [J/K]
MB	abbreviation for Maxwell-Boltzmann in reference to the velocity distribution
MD	abbreviation for molecular dynamics
m_g	gas molecule mass [kg]
m_s	surface atom (or cube) mass [kg]
R	morse potential parameter [nm]
r_{ij}	gas-surface interatomic spacing [nm]
SC	abbreviation for soft cube model
TAC	abbreviation for thermal accommodation coefficient
T_g	gas temperature [K]
T_s	surface temperature [K]
T_θ	Debye temperature [K]
u	normal gas molecule velocity [m/s]
u_D	gas molecule escape velocity [m/s]
$U_{ij}(r_{ij})$	gas-surface interatomic potential [J]
$\boldsymbol{v}$	gas molecule velocity vector [m/s]
v	in-plane gas molecule velocity [m/s]
v_s	surface atom (or cube) velocity [m/s]
v_t	tangential gas molecule velocity [m/s]
w	out-of-plane gas molecule velocity [m/s]
WA	abbreviation for washboard model
α	total translational TAC
α_i	in-plane TAC
α_n	normal TAC
α_o	out-of-plane TAC
α_t	tangential TAC
β_T	inverse most probable speed [m/s]
ϕ	angle between normal and tangential gas molecule velocities [°]
γ	corrugation angle, WA model [°]
γ_i	in-plane corrugation angle, WA model [°]
γ_m	maximum corrugation angle, WA model [°]
γ_o	out-of-plane corrugation angle, WA model [°]
μ	mass ratio, $\mu = m_g/m_g$
θ	angle between tangential components of gas molecule velocity [°]
τ	temperature ratio, $\tau = T_g/T_s$
ζ	initial phase of motion, SC model [°]
$\langle\cdot\rangle$	denotes an average

the potential well depth, meaning that direct scattering is more probable than trapping/desorption on the surface. In the context of TiRe-LII, TACs are usually inferred from pyrometrically-inferred cooling rates of laser-heated nanoparticles having a known size distribution, most often from *ex situ* analysis [8,17,18,32–34]. Unfortunately, the accuracy of LII-inferred TACs is limited by uncertainty in the spectroscopic and heat transfer model parameters, including the radiative and thermodynamic properties of the nanoparticles and the *ex situ* nanoparticle sizes. To address this shortcoming, Daun et al. [23,24,35–37] and Sipkens et al. [27] used MD simulations to estimate the TAC under TiRe-LII conditions. Fig. 1a shows that MD-simulated TACs for Si-He [27] are consistent with the trends in experimental and MD studies in regards to T_s. Fig. 1b shows that MD [23,24,27,35,37] also captures how TACs derived from TiRe-LII measurements vary with μ [8,17,18,27,32,33].

The broad agreement between MD- and experimentally-derived TACs highlights the robustness of the MD-derived estimates and suggests that a classical conceptualization of gas-surface scattering is sufficient to capture the key physical processes important to the TAC under these conditions. Nevertheless, the complexity of the many-body interactions that underlie a MD simulation can preclude a deeper understanding of the basic physics involved in these interactions. For example, while one may conclude from Fig. 1b that the TAC increases monotonically with μ, the potential well-depth also generally increases with gas molecular mass due to the increased polarizability of larger molecules, and the MD simulations by themselves do not provide any way to distinguish how these parameters effect the TAC [36,37]. To this end, we apply simpler cube models, specifically the hard cube (HC); soft cube (SC); and washboard (WA) models, as a form of model reductionism to discern trends in MD-predicted TACs at temperatures exceeding 1500 K. Although cube models are often dismissed as obsolete compared to more accurate MD simulations, variations between the cube model predictions and a comparison to more accurate but complex MD simulations provides physical insight that can be used to interpret trends in key parameters. The HC model, which is the most basic, consists of an oscillating cube and considers normal momentum conservation and energy transfer between the surface and the gas molecule. The SC model "softens" the gas-surface interaction via a spring connecting the surface cube to the rest of the lattice, allowing the gas molecule to transfer some of its energy to the surrounding lattice. The WA model expands on the HC model by introducing a corrugation effect, which can lead to backscatter and interactions between the translational energy modes of the gas molecules. While other, more complex, cube models are available [38–40], we restrict our analysis to the HC, SC, and WA models since our interest is in elucidating key physical trends through model reductionism and not developing accurate predictions to be used in calculating heat transfer rates. The present study is also limited to monatomic gas molecules, although some cube models have been adopted to consider diatomic gas molecules [38,39].

The paper starts with an overview of the velocity distributions and coordinate systems used in the analyses, along with a formal definition of the TAC and its various modes. The subsequent sections present the cube model results, along with a discussion of the sensitivity of the TAC to uncertain model parameters. Finally, the cube model results are compared to the results of MD simulations on Si-He, generated following the procedure described in Sipkens et al. [27]. The results elucidate the physics behind the key trends observed in MD simulations. In particular, the HC model captures trends in the TAC with respect to mass and temperature ratios. The SC model predictions are closer to MD simulations because the SC model accounts for deformation work done by the gas molecule on the surface atoms and incorporates the surface frequency/lattice vibrations. The introduction of corrugation in the WA model allows for in-plane and out-of-plane trends that are more consistent with MD simulations.

2. Velocity distributions and energy transfer

2.1. Incident conditions

The gas molecular velocity, $\mathbf{v} = [u, v, w]^T$, is defined relative to a coordinate system aligned with the surface, such that u is normal

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