



DESIGN OF SOLID-GAS INTERFACES FOR ENHANCED THERMAL TRANSFER

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14. ABSTRACT
Using the molecular dynamics simulation and related analysis we investigated the thermal accommodation coefficient (TAC) and the momentum accommodation coefficient (MAC) to quantify the solid-gas energy and momentum exchange efficiencies. We determined the effects of individual interfacial parameters including, (i) solid-gas interaction strength, (ii) gas-solid atomic mass ratio, (iii) solid elastic stiffness, and (iv) temperature, on TAC and MAC at solid surfaces in contact with monoatomic and diatomic gases. We demonstrated that the TAC and MAC can be significantly enhanced by proper surface modifications. Specifically, for metal surfaces modified with organic self-assembled monolayers (SAMs), both TAC and MAC are close to its theoretical maximum and are essentially independent from the details of the SAM-gas interactions characteristics. Our work provided clear guidelines for solid surface modification enabling efficient energy exchange at the solid-gas interface and generated an extensive database for the TAC and MAC which can be utilized in the design of gas cooling systems critical in thermal management of a wide range of of a wide range of active electrical and mechanical components used in the Air Force hardware.

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Abstract:

This project using the molecular dynamics simulation and related analysis we investigated the thermal accommodation coefficient (TAC) and the momentum accommodation coefficient (MAC); two fundamental parameters quantifying the solid-gas energy and momentum exchange efficiencies. In particular we determined the effects of individual interfacial parameters including, (i) solid-gas interaction strength, (ii) gas-solid atomic mass ratio, (iii) solid elastic stiffness, and (iv) temperature, on TAC and MAC at solid surfaces in contact with monoatomic and diatomic gases.

Guided by the determined relationships and parametric dependencies we proposed and demonstrated that the TAC and MAC can be significantly enhanced by proper surface modifications. Specifically, for metal surfaces modified with organic self-assembled monolayers (SAMs), both TAC and MAC are close to its theoretical maximum and are essentially independent from the details of the SAM-gas interactions characteristics. The analysis of the simulation results indicates that much softer and lighter SAMs, compared to the bare metal surfaces, are responsible for the greatly enhanced TAC, and the greatly enhanced MAC is mainly due to the fact that SAMs are much rougher than the bare metal surfaces.

In addition to offering a fundamental understanding on how individual parameters affect the nature of gas-solid collisions and providing a clear guideline for solid surface modification allowing to reach theoretical limits for the thermal energy exchange at the solid-gas interface, we generated an extensive database for the TAC and MAC which will be utilized in the design of gas cooling systems critical in thermal management of a wide range of active electrical and mechanical components used in the Air Force hardware.

Our modeling results have resulted in multiple publications including in Applied Physics Letters, Physical Review E, International Journal of Heat and Mass Transfer and Journal of Chemical Physics.

1. Background and motivation

Convective heat transfer in rarefied gases is of great importance to the thermal management of microelectronic devices [1-3], microelectromechanical systems (MEMS) based devices [4], and aircraft flying at high altitudes [5,6]. The degree of rarefaction of a gas can be described by the Knudsen number $Kn = \lambda/L$, where λ is the mean free path of gas molecules and L is a characteristic dimension. When λ is comparable to or smaller than the microstructural feature size of the cooling device, the energy and momentum transfer at solid-gas interfaces has strong affect the overall heat transfer efficiency.

In order to investigate the heat transfer to a body in a rarefied gas, the well-established continuum theories must be modified to account for the velocity slip and temperature jump at the solid wall [4-6]. According to the gas kinetic theory [7,8], the velocity-slip and temperature-jump boundary conditions can be incorporated by introducing two parameters called momentum accommodation coefficient (MAC), defined as the fraction of gas molecules reflected diffusely from the solid surface, and thermal accommodation coefficient (TAC), defined as the fraction of gas molecules incident on the surface scattered in thermal equilibrium with the surface.

Despite the fact that the subjects of the TAC and MAC have over a century-long history of investigation, presently no quantitative theory exists and there are only semi-quantitative or empirical formulas available to fit experimental data [9]. These formulas have limited applicability to a wide range of gas-solid interfaces and temperatures. Moreover, the role of individual parameters is often difficult to determine in experiments [6]. To understand and quantify the role of individual interfacial parameters and to determine how these parameters affect the nature of gas-solid collisions and the value of the TAC and MAC, we resorted to molecular dynamics (MD) simulations and a suite of molecular-level thermal characterization techniques.

Molecular simulations are uniquely positioned to explore the mechanism behind the energy and momentum transport at solid-gas interfaces. In the past decade, the MD simulation has been utilized to study the TAC and MAC of noble gases on various solid surfaces [10-12]. However, each of these work only investigated one or two factors that influence TAC or MAC. Moreover, a systematic study of effects of various parameters on the TAC and MAC of diatomic or polyatomic gases is not available. In this project, we carried out a systematic study of the effects of various parameters of importance, including the solid-gas interaction strength, the gas-solid mass ratio, and the temperature and elastic modulus of solid on the TAC and MAC. In addition to study the accommodation coefficients of monoatomic gases on solid surfaces, we also investigated the TAC and MAC of diatomic gases on thermal and momentum accommodation of various gases. Through the extensive MD simulations, we generated a database for TAC and MAC and provided a fundamental understanding of the nature of thermal and momentum accommodation for monoatomic and diatomic molecules. Based on this understanding, we designed solid surfaces functionalized with organic self-assembled monolayers (SAMs) and demonstrated associated significant improvement of the thermal and momentum exchange efficiency.

2. Scientific approach for determination of TAC and MAC.

2.1. Theory.

In the case of monoatomic gases TAC is defined by [9]

$$\alpha_T = (T_r - T_i)/(T_s - T_i) \quad (1)$$

where T_i and T_r are the temperatures of incident and reflected gas atoms, respectively, and T_s is the solid surface temperature. $\alpha_T = 1$ means there is a complete thermal equilibration of the incident gas stream with the solid. In the case of diatomic gases, the TAC can be also calculated by Eq. (1), if the diatomic molecule can be approximated as a classical rigid rotor. For diatomic gases, we can further calculate the translational and rotational temperatures of gas molecules, thus obtain the TACs for translational and rotational molecular motions.

In the temperature jump regime ($0.01 < \text{Kn} < 0.1$), TAC relates to the solid-gas interfacial thermal conductance G_K by [8]

$$G_K = f k_B N \alpha_T / (2 - \alpha_T) \quad (2)$$

where $f = 4$ for a monoatomic gas and $f = 6$ for a diatomic gas, k_B is the Boltzmann constant, and N is collision rate per unit area. The collision rate is a function of pressure, P , temperature, T , and the atomic mass m , and it is given by [8]

$$N = P / \sqrt{2\pi m k_B T} \quad (3)$$

The interfacial thermal conductance can be readily obtained from non-equilibrium MD (NEMD) simulations using

$$G_K = q / \Delta T \quad (4)$$

where q is the heat flux across the solid-gas interface, and ΔT is a temperature jump at the solid-gas interface. Hence, the relation between G_K and α_T given by Eq. (2) can be used to verify the consistency of the TAC calculated directly by Eq. (1) and via Eq. (2).

Similar to Eq. (1), the equation to calculate tangential-MAC is [13]

$$\alpha_v = (v_{x,r} - v_{x,i}) / (v_{x,s} - v_{x,i}) \quad (5)$$

where $v_{x,i}$ and $v_{x,r}$ are the tangential velocities of incident and reflected gas molecules, respectively, and $v_{x,s}$ is the tangential velocity of solid surface. $\alpha_v = 1$ means all gas molecules are diffusely scattered by the surface. If $v_{x,s} = 0$ which is the case in our MD simulation, Eq. (5) can be simplified to Eq. (6).

$$\alpha_v = 1 - v_{x,r} / v_{x,i} \quad (6)$$

According to Eq. (6) $v_{x,r}$ is linearly proportional to $v_{x,i}$ if the macroscopic velocity of the solid is zero. This relation is utilized in our MD simulations to calculate the tangential-MAC.

2.2. MD simulations.

The typical model system consisted of a solid metal (Pt or Au) slab in contact with Ar or N₂ gas, as depicted in Fig. 1(a). The embedded-atom-method (EAM) potential [14] was used for realistic description of Au-Au interactions. The Lennard-Jones (LJ) 12-6 potential, with parameters $\sigma = 3.41 \text{ \AA}$ and $\varepsilon = 10.3 \text{ meV}$ [15], is employed for Ar-Ar interactions. The N₂ molecule with a bond length of 1.10 \AA [16] is considered as a rigid rotor in the MD simulation. The LJ potential, with parameters $\sigma = 3.31 \text{ \AA}$ and $\varepsilon = 3.21 \text{ meV}$ [17], is employed for N-N interactions between molecules. In the case of Au surfaces functionalized with SAMs, 1-octanethiolate [-S-(CH₂)₇-CH₃] chains are covalently bonded to Au surface. The interatomic interactions for SAM molecules are described by the Hautman-Klein united atom (UA) model [18]. LJ potentials are used for non-bonded interactions in SAM molecules in the UA model. The Koike-Yoneya bond stretching potential [19] is included in the UA potential to take into account the C-C and C-S bond stretching motions. The Au-S interactions are modeled by the Morse

potential [1,20]. LJ potentials for interactions between Au and other atoms in SAMs are taken from the universal force field (UFF) [21].

To calculate the TACs and MACs using Eq. (1) and Eq. (6), we set an imaginary plane 11 Å (cutoff distance) away from the solid surface. The small distance between the plane and surface ensures that the collisions between gas atoms moving from the plane to the solid surface and back are rare by comparison with the collisions with the solid. The incident (or reflected) gas molecules pass through the imaginary plane indicating the start (or finish) of the energy and momentum exchange process. The temperature of incident (or reflected) gas molecules is obtained by dividing the average kinetic energy of the incident (or reflected) molecules by $2k_B$ for monoatomic gases, and by $3k_B$ for diatomic gases [8]. For diatomic gases, we further divide the kinetic energy into translational and rotational kinetic energies, and thus calculate the translational and rotational components of the TACs.

To calculate MACs, we monitored the tangential velocity of incident molecules ranging from -400 m/s to 400 m/s. Out of this range, the statistics is poor within the finite simulation length. For each incident tangential velocity $v_{x,i}$, we calculated the average reflected tangential velocity $v_{x,r}$. To get good statistics, $v_{x,i}$'s are divided into bins with the width of 6 m/s. The slope of linear fit of $v_{x,r}$ vs. $v_{x,i}$ was used to determine MAC based on Eq. (6). The uncertainties are determined from the analysis of eight independent simulation runs.

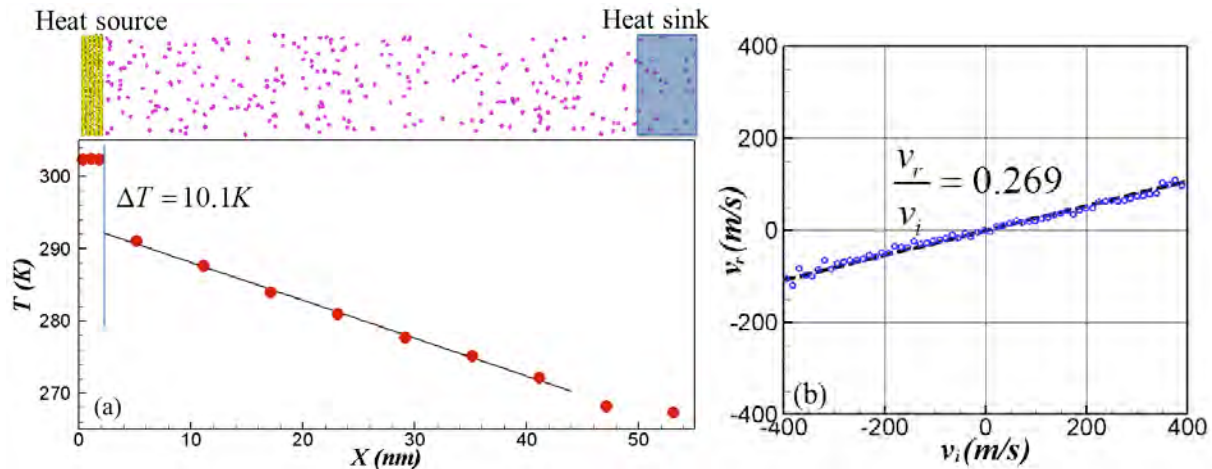


FIG. 1. (a) A snapshot of solid-gas system and the steady state temperature profile. Due to the symmetry of the system, only half of the simulation box is shown. (b) The reflected tangential velocity as a function of the incident tangential velocity. The dashed line is a linear fit to the simulation data.

3. Research results.

3.1. Thermal and momentum accommodation of monoatomic gases on solid surfaces.

3.1.1. Effects of solid-gas interaction strength on TAC.

Gas atoms exchange thermal energies and momenta with solid surfaces through solid-gas interactions/collisions. If gas atoms are adsorbed on the surface, the solid-gas interaction time will be much longer than that in the case of direct inelastic scattering. Longer interaction time leads to the more thorough thermalization of gas atoms at the surface, a higher accommodation coefficient, and thus, a higher G_K .

The dependence of TAC on solid-gas binding energy parameter, ϵ_{sf} , is shown in Fig. 2. At low interaction strength TAC is low as the atoms collide with the surface with little energy exchange. As the bonding is increases we observed that upon collision most gas atoms are adsorbed, thermally equilibrated over 100 ps or more with the surface and desorb. This leads to the TAC close to the theoretical maximum of 1. This result is consistent with the findings in Ar + Pt(111) molecular beam scattering experiments and simulations which show a complete thermalization of Ar requires over 100 ps [23].

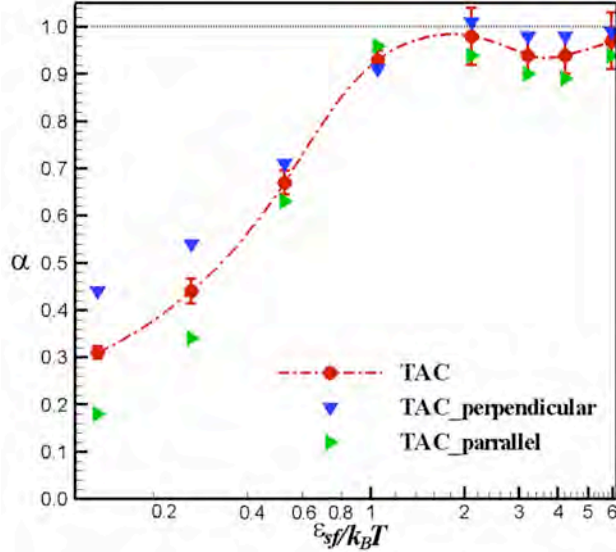


FIG. 2. Thermal accommodation coefficient (total, perpendicular component and parallel component) as a function of solid-gas binding strength ϵ_{sf} . The dash-dot line is used to guide the eye.

3.1.2 The mass effect on the TAC and MAC of a monoatomic gas.

The mass effect on TAC is presented in Fig. 3 (a). At small bonding increased mass of the gas atoms leads to increased energy exchange efficiency as the gas atom mass is better matching solid atom mass. When the trapping-desorption dynamics dominates for stronger interactions, the TACs are essentially mass independent and close to the theoretical maximum ($\alpha_T = 1$). The mass effect on the MAC is shown in Fig. 3(b). Similar to the TAC, we find the MAC increases with ϵ_{sf} . However, the MAC is essentially mass independent for a given ϵ_{sf} . The result indicates that the mass ratio is not a critical factor affecting the MAC.

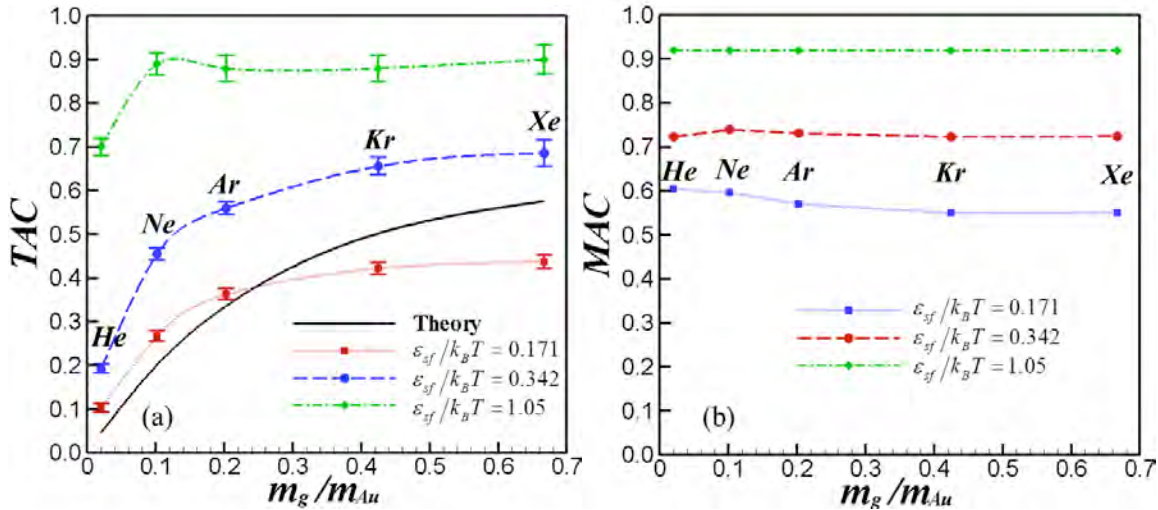


FIG. 3. The TAC and MAC as a function of the gas-solid mass ratio at 300 K. (a) The TAC on a bare Au surface. The mass of solid atom is fixed. The mass of gas atom varies from the mass of He to the mass of Xe. The solid line represents the prediction from the hard-sphere model. (b) Same as (a) but for the MAC. The solid and dashed lines connecting simulation data are used to guide the eye (same for the following figures).

3.2.3 The effect of solid elasticity on TAC and MAC of a monoatomic gas.

The elastic modulus (Young's modulus), E , of solid Au is about 78 GPa [24]. Many other materials such as Pt and W are much stiffer than Au. To study the effect of solid elasticity, we tune the prefactor in the EAM potential from 0.3 to 5. Since the elastic modulus is proportional to the prefactor, E of the solid varies from 23.4 GPa to 390 GPa.

As shown in Fig. 4(a), the TAC decreases almost linearly with increasing E . When E is small, the gas atoms collide essentially with individual solid atoms since the solid atoms are weakly connected to each other. As E gets greater, solid atoms are more tightly bonded to each other. In this case, the gas atoms collide with multiple atoms, i.e., effectively a heavier solid atom, which results in larger mass mismatch and a smaller TAC. The MAC is about 0.7 and has little variability with the solid modulus, except for the very E limit where surface becomes quite rough due to a large amplitude of thermal motion associated with soft solid-solid atomic bonds.

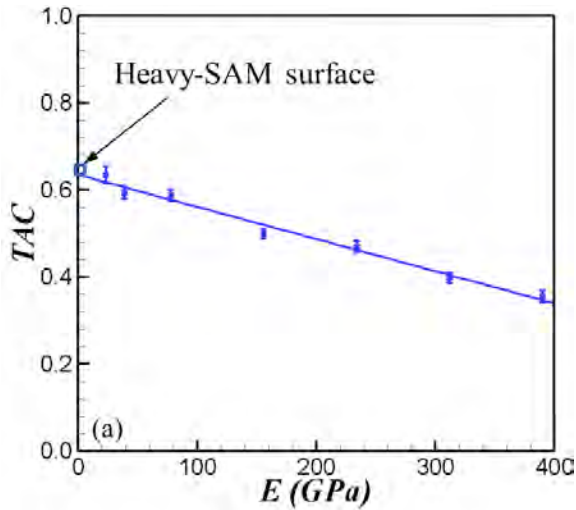


FIG. 4. The TAC on a bare solid surface as a function of elastic modulus. Heavy-SAM surface result is also shown and it corresponds effectively to the collision with individual unbonded atoms.

3.2.4 Significant enhancement of TAC and MAC by functionalizing solid surface with organic SAMs.

The aforementioned parametric study demonstrated that the improvement of thermal exchange efficiency at the solid-gas interface can be achieved by improving the mass matching between gas atoms and surface solid atoms,

reducing the solid elasticity, and associated increase of the surface roughness.

These results led us to the hypothesis that introduction of soft organic molecular layer (i.e. SAM in our studies) can significantly improve energy and mass transfer. Indeed, As shown in Fig. 5, TAC at the SAM surface is rather independent from the gas-solid interaction strength and close to 1. This shows that the highly efficiently thermal energy exchange between the solid and gas can be always achieved by modifying a bare Au surface with SAMs. The MAC (not shown) is also improved from 0.7 value characterizing bare solid surface to ~ 0.9 .

3.3. Thermal and momentum accommodation of diatomic gases on solid surfaces.

As shown in Fig. 6(a), the TAC for N_2 on a bare Au surface increases with ϵ_{sf} . When the Au surface is functionalized with SAMs, the TAC is significantly enhanced and also increases with ϵ_{sf} . These results are similar to what we found on the TAC of Ar. The difference is the TAC of Ar on a SAM surface is essentially independent of ϵ_{sf} . This difference may come from the relatively lower thermal accommodation of rotational kinetic energy α_{rot} of N_2 . For instance, with $\epsilon_{sf}/k_B T = 0.171$ α_{tr} of N_2 increases from 0.40 (on the bare Au surface) to 0.83 (on the SAM surface) and α_{rot} increases from 0.29 to 0.59. The result shows the rotational motion of N_2 is difficult to fully thermalize during a collision even with the soft SAM surface. As was in the case for Ar gas, all MACs obtained on the SAM surface are high and within a narrow range of 0.86 ± 0.05 , while on bare surfaces values of MACs are much smaller.

The role of other parameters, such as solid elastic constant and gas molecule mass is similar in the cases of diatomic and monoatomic gases. Also, in all cases the rotation energy accommodation is less efficient than the translational one.

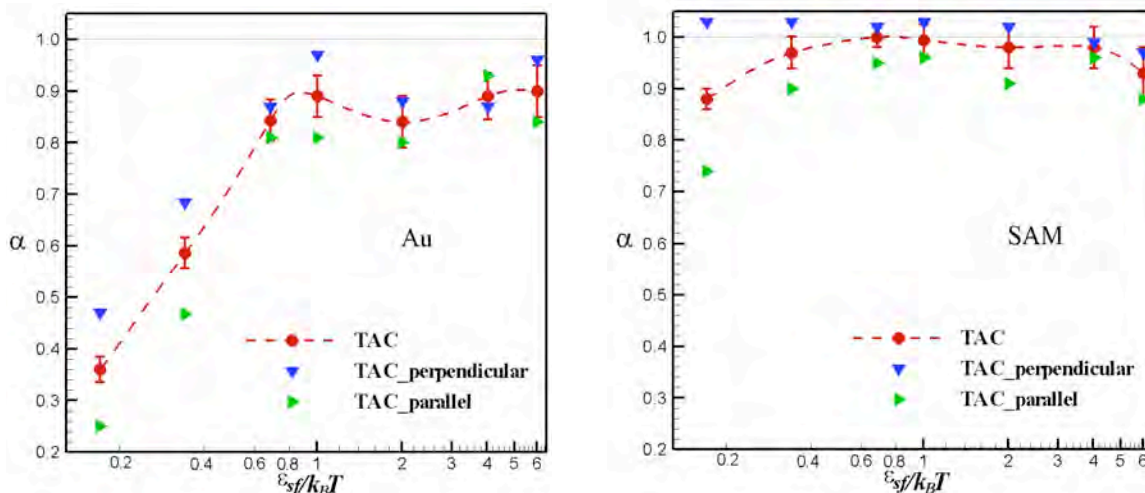


FIG. 5. TAC as a function of solid-gas interaction strength ϵ_{sf} for (a) Ar-Au system and (b) Ar-Au/SAM system.

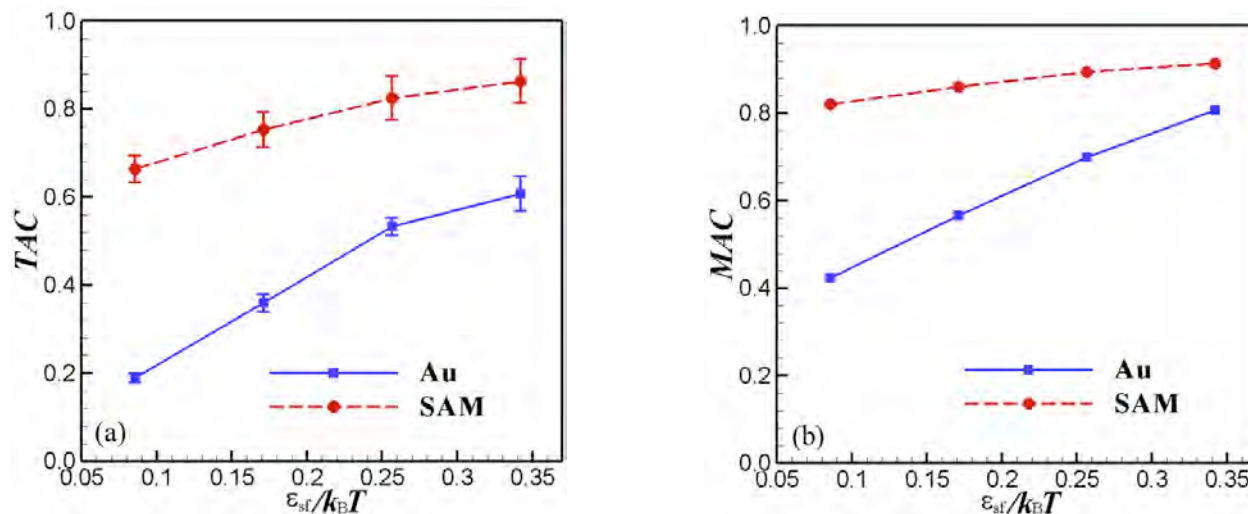


FIG. 6. (a) The TAC and (b) the MAC of N_2 on a bare Au and a SAM surface as a function of solid-gas interaction strength.

4. Summary and conclusions.

The TAC and MAC of monoatomic and diatomic gases on a bare solid surface were calculated through extensive MD simulations. The effects of the gas-solid mass ratio m_g/m_s , the solid-gas interaction strength ϵ_{sf} , the temperature T , and the solid elasticity E were studied. The following results were obtained.

- (i) The TAC and MAC generally increase with the dimensionless quantity $\varepsilon_{sf}/k_B T$, which implies an increase of solid-gas interaction strength has about the same effect as a decrease of temperature. The results are associated with the transition from collision type scattering to adsorption-desorption types of scattering.
- (ii) On a SAM surface, the TAC of a monoatomic gas reaches a maximum when the gas atom has a perfect mass matching with the surface atom (sum of the three pseudo-atoms closest to the SAM surface). Such a maximum TAC is not observed for a diatomic gas on a SAM surface, which is due to rotational motions being more difficult to fully thermalize with a SAM surface.
- (iii) The MAC is essentially independent of the gas-solid mass ratio. A key factor that affects the MAC is solid surface structure. The MAC is much higher on a disordered and rough surface than on an ordered smooth surface.
- (iv) As the solid modulus increases, the TAC decreases.

Based on the above results we proposed and demonstrated that surfaces functionalized with SAMs has greatly improved TAC and MAC across a wide range of system conditions and parameters and provides a robust approach to development of more efficient materials for gas-solid energy exchangers

Our results also indicate that solid surfaces with larger roughness, structural and chemical defects will lead to more diffuse scattering of gas molecules and improved energy and momentum exchange. Consequently, development of high-quality, smooth interfaces is not desired in this case, not only due to synthesis challenges, but also due to the fact of their poor performance.

5. Publications supported by this project.

1. Zhi Liang, William Evans, Tapan Desai and Pawel Keblinski, "Improvement of heat transfer efficiency at solid-gas interfaces by self-assembled monolayers" Applied Physics Letters **102**, 061907 (2013).
2. Zhi Liang, William Evans, and Pawel Keblinski, "Equilibrium and nonequilibrium molecular dynamics simulations of thermal conductance at solid-gas interfaces" Physical Review E **87**, 022119 (2013).
3. Zhi Liang and Pawel Keblinski, "Parametric studies of the thermal and momentum accommodation of monoatomic and diatomic gases on solid surfaces" International Journal of Heat and Mass Transfer **78**, 161 (2014).
4. Zhi Liang and Pawel Keblinski, "Slip length crossover on a graphene surface" Journal of Chemical Physics **142**, 134701 (2015).
5. Zhi Liang and Pawel Keblinski, "Coalescence-induced jumping of nanoscale droplets on super-hydrophobic surfaces" (submitted).

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Pawel Keblinski

Program Manager

The AFOSR Program Manager currently assigned to the award

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Abstract

Using the molecular dynamics simulation and related analysis we investigated the thermal accommodation coefficient (TAC) and the momentum accommodation coefficient (MAC); two fundamental parameters quantifying the solid-gas energy and momentum exchange efficiencies. In particular we determined the effects of individual interfacial parameters including, (i) solid-gas interaction strength, (ii) gas-solid atomic mass ratio, (iii) solid elastic stiffness, and (iv) temperature, on TAC and MAC at solid surfaces in contact with monoatomic and diatomic gases.

Guided by the determined relationships and parametric dependencies we proposed and demonstrated that the TAC and MAC can be significantly enhanced by proper surface modifications. Specifically, for metal surfaces modified with organic self-assembled monolayers (SAMs), both TAC and MAC are close to its theoretical maximum and are essentially independent from the details of the SAM-gas interactions characteristics. The analysis of the simulation results indicates that much softer and lighter SAMs, compared to the bare metal surfaces, are responsible for the greatly enhanced TAC, and the greatly enhanced MAC is mainly due to the fact that SAMs are much rougher than the bare metal surfaces.

In addition to offering a fundamental understanding on how individual parameters affect the nature of gas-

solid collisions and providing a clear guideline for solid surface modification allowing to reach theoretical limits for the thermal energy exchange at the solid-gas interface, we generated an extensive database for the TAC and MAC which will be utilized in the design of gas cooling systems critical in thermal management of a wide range of active electrical and mechanical components used in the Air Force hardware.

Our modeling results have resulted in multiple publications including in Applied Physics Letters, Physical Review E, International Journal of Heat and Mass Transfer and Journal of Chemical Physics.

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2. Zhi Liang, William Evans, and Pawel Keblinski, "Equilibrium and nonequilibrium molecular dynamics simulations of thermal conductance at solid-gas interfaces" Physical Review E 87, 022119 (2013).
3. Zhi Liang and Pawel Keblinski, "Parametric studies of the thermal and momentum accommodation of monoatomic and diatomic gases on solid surfaces" International Journal of Heat and Mass Transfer 78, 161 (2014).
4. Zhi Liang and Pawel Keblinski, "Slip length crossover on a graphene surface" Journal of Chemical Physics 142, 134701 (2015).
5. Zhi Liang and Pawel Keblinski, "Coalescence-induced jumping of nanoscale droplets on super-hydrophobic surfaces" (submitted).

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Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

	Starting FY	FY+1	FY+2
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