ADSORPTION-CONTROLLED THERMAL DIODE: NONEQUILIBRIUM MOLECULAR DYNAMICS SIMULATION

Tadeh Avanessian, and Gisuk Hwang
Department of Mechanical Engineering, Wichita State University

Wichita State University GRASP Symposium, April 29th 2016

Motivation, Challenges, and Objectives

Motivation

- Optimal thermal management systems are crucial to many applications in manufacturing, electronics, automotive, aerospace, and energy systems.
- Thermal energy flow often needs to be controlled in direction for the desired flow control.

Challenges

- Thermal flow control systems are rare.
- They have poor steady state performance, slow transient response, and difficult manufacturing process.

Objectives

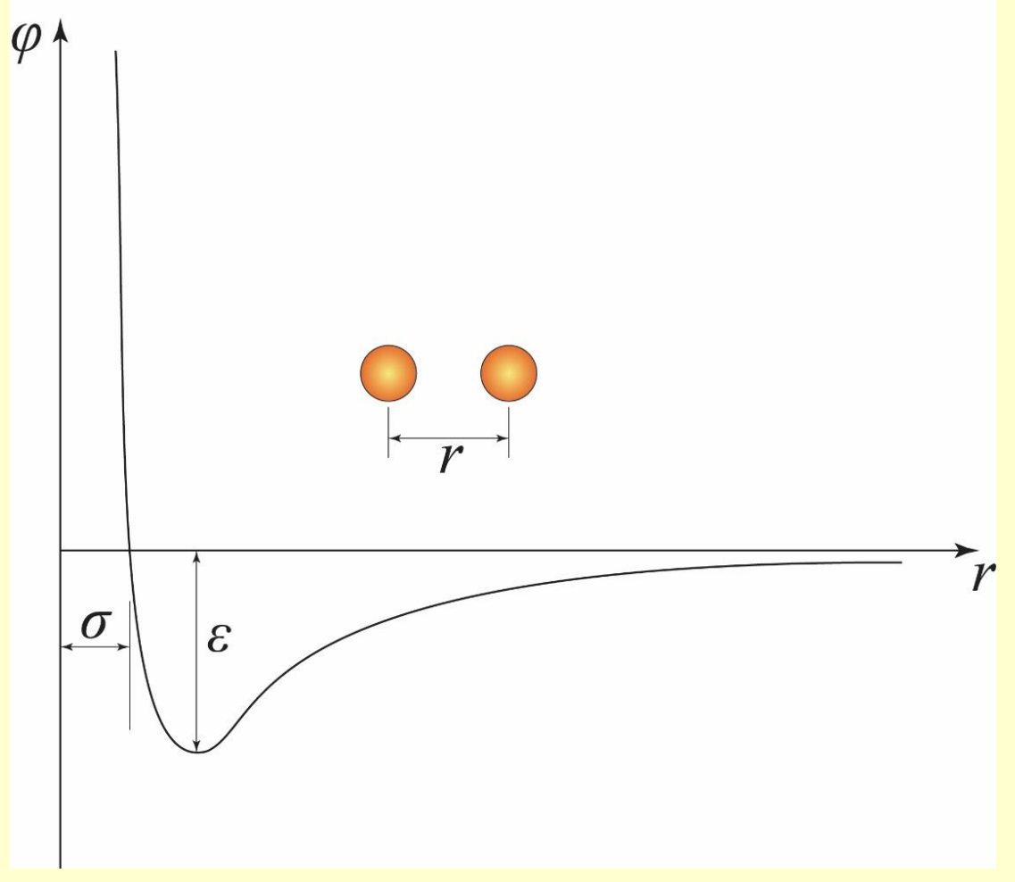
- Achieving adsorption-controlled thermal rectification in a gas-filled nanogap with heterogeneous solid-gas interactions as a new class of fast and efficient thermal diodes.

Background: Molecular Dynamics Simulation

Inter-atomic Interaction:

Ar – Ar and Ar - surface particles:

$$\varphi_{ij} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

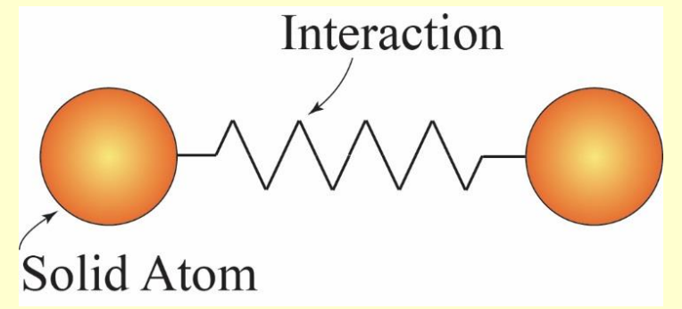


solid – solid interaction:

$$\varphi_{ij} = k\left(r_{ij} - r_0\right)^2$$

k = 67.360 kcal/mol-Å^2

r_0 = 2.77 Å



Background: Thermal Accommodation Coefficient

Thermal Accommodation Coefficient (TAC)

$$a_T = \frac{\langle q_{f,z}\rangle - \langle q_{f,z}\rangle'}{\langle q_{f,z}\rangle - \langle q_{f,z}(T_s)\rangle}$$

$a_T \rightarrow 0$: fluid particle retains its temperature after reflection (no interaction)

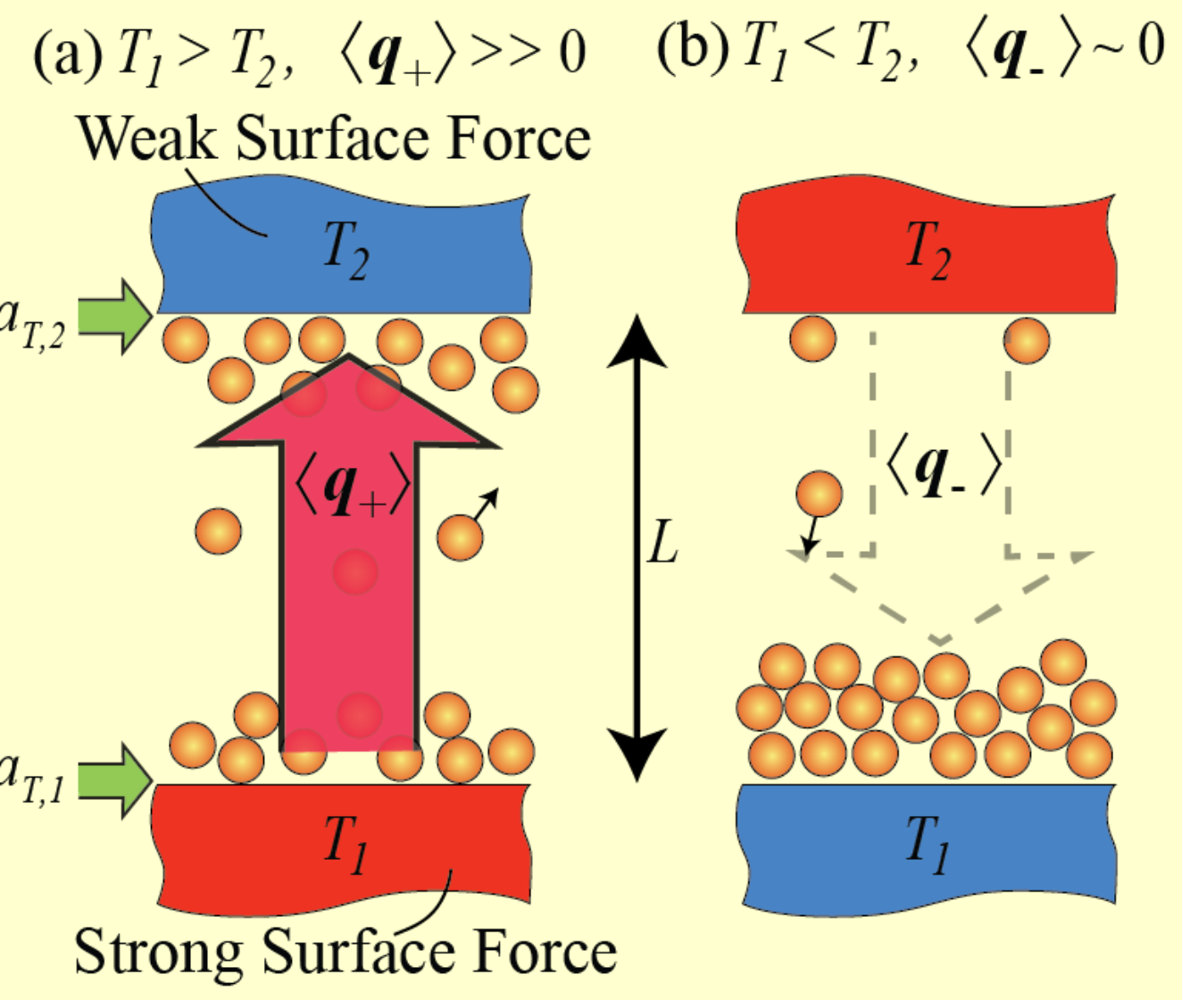
$a_T \rightarrow 1$: fluid particle has the wall temperature after reflection (large interaction)

Degree of Rectification

$$R = \frac{|\boldsymbol{q}_+| - |\boldsymbol{q}_-|}{|\boldsymbol{q}_-|}$$

Thermal rectification is achieved when:

$<\boldsymbol{q}_+> \; >> \; <\boldsymbol{q}_->$


(a) $T_1 > T_2$, $\langle \boldsymbol{q}_+ \rangle >> 0$ (b) $T_1 < T_2$, $\langle \boldsymbol{q}_- \rangle \sim 0$

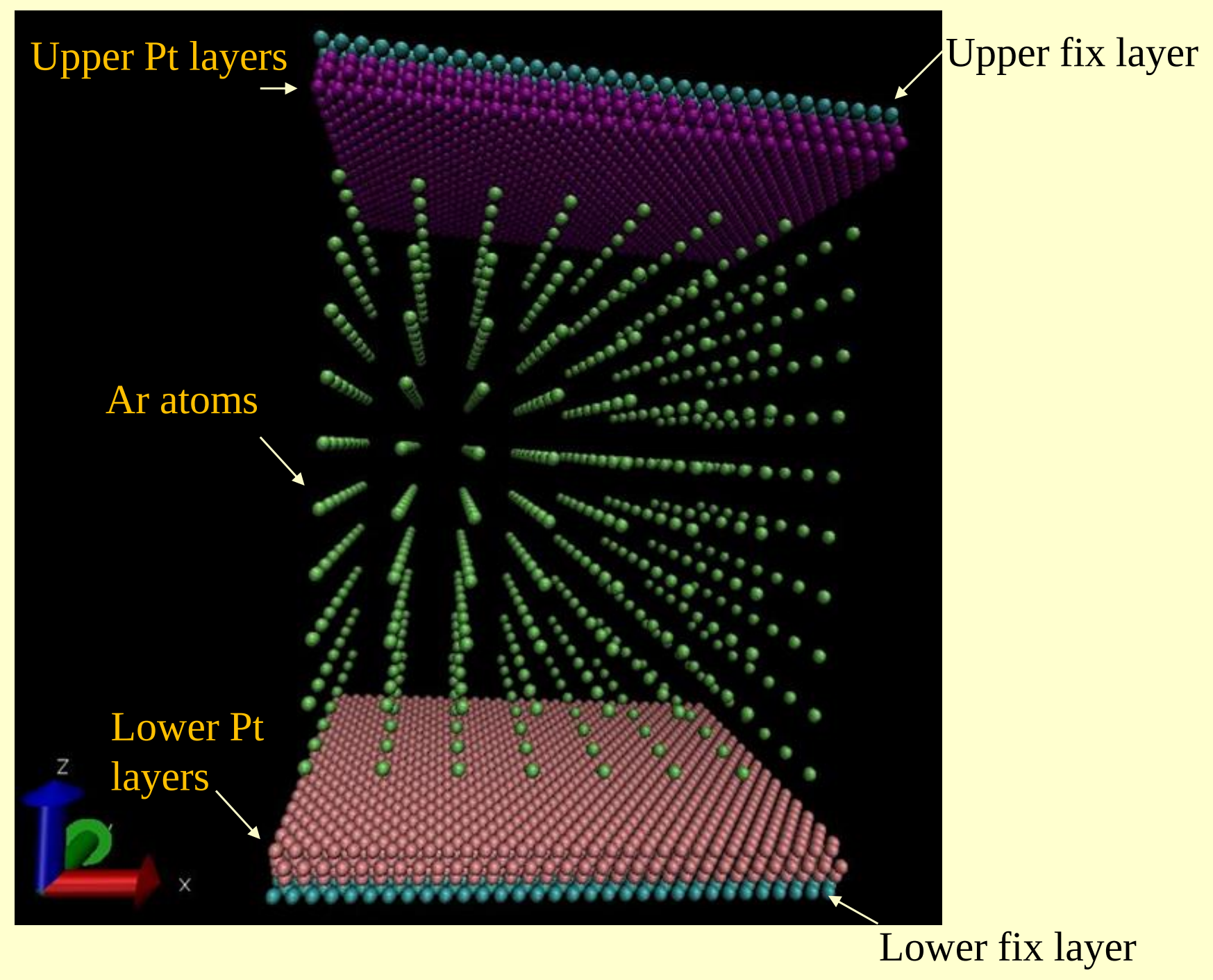
Methodology: Interatomic Parameters, Nanogap Geometry, and Heat Flux Calculation

Lennard-Jones potential parameters for the interacting atoms

Interacting Atoms	ε_{ij} (kcal/mol)	σ_{ij} (Å)
Ar - Ar	0.2403	3.405
Ar – Pt (strong surface)	ε_1 = 0.1573	3.09
Ar – weak surface	$\varepsilon_2 = \varepsilon^* \times \varepsilon_1$	3.09

ε^* = 0.1 or 0.5 (in this study)

$$<q_{k,g}> = \frac{1}{V}\left[\sum_{i=1}^{N}\frac{1}{2}m_i u_i^2 u_{i,z} + \sum_{i=1}^{N}\sum_{j>1}^{N}\varphi_{ij}u_{i,z} - \sum_{i=1}^{N}\sum_{j>1}^{N}(\boldsymbol{r}_{ij}\cdot\boldsymbol{F}_i)u_{i,z}\right],$$



Results and Discussions: Heat Flux, *R*, and Pressure

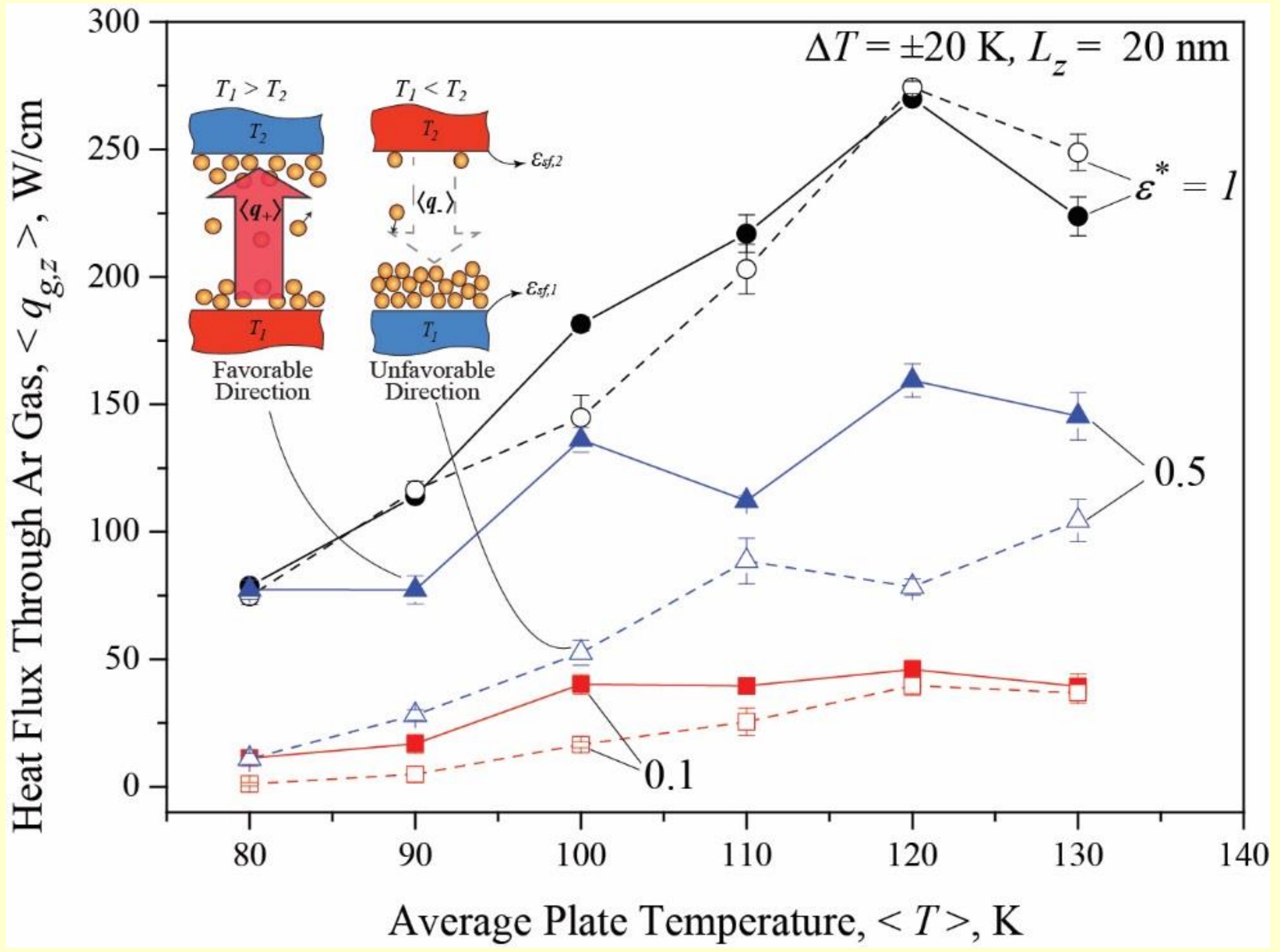


Figure 1. Heat flux through the nanogap in positive and negative directions for ε^* = 0.1, 0.5, and 1.0

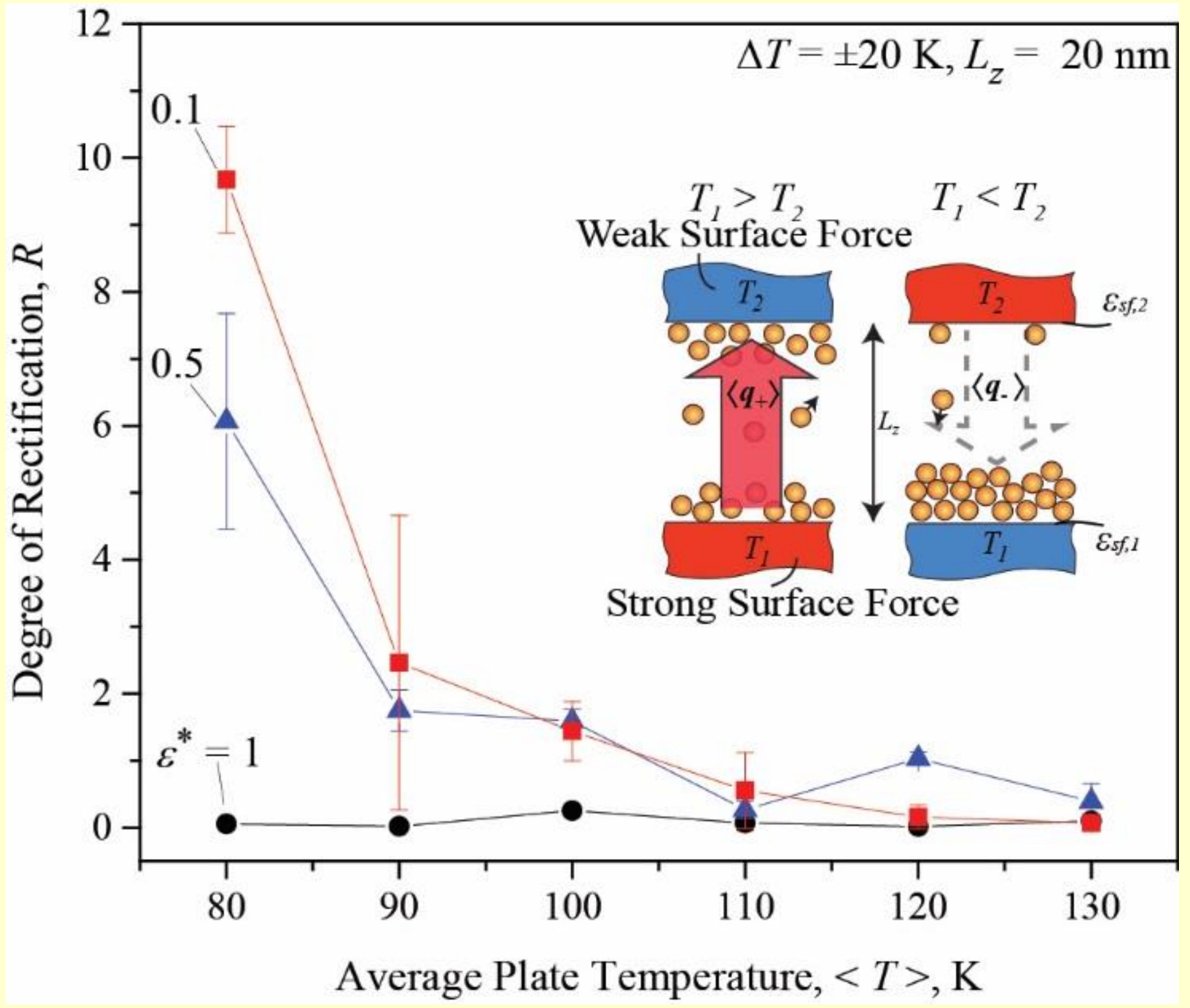


Figure 2. The degree of rectification (R) for ε^* = 0.1, 0.5, and 1.0

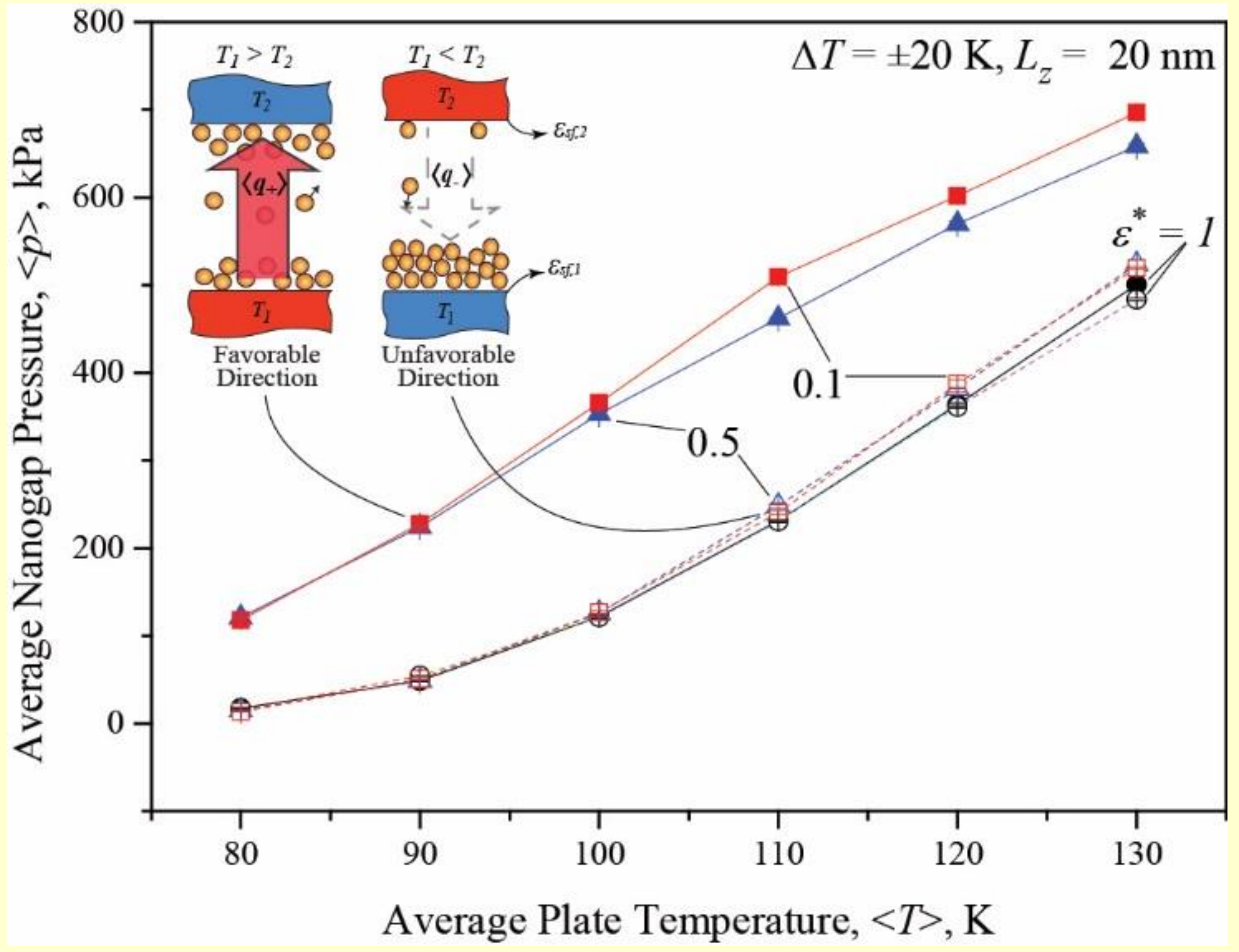


Figure 3. Nanogap pressure in positive and negative directions for ε^* = 0.1, 0.5, and 1.0

- For ε_{sf}^* = 1, no significant difference between $<q_+>$ and $<q_->$ is found due to the symmetric surface interaction (Figure 1)
- For ε_{sf}^* = 0.1 and 0.5, the heat flux in the favorable direction is much higher than that in reverse direction, due to the asymmetric surface interaction, i.e., adsorption-controlled TAC (Figure 1).
- For ε_{sf}^* = 1.0, the $R \sim 0$ as predicted, i.e., no thermal diode effect and symmetric heat flux (Figure 2).
- For ε_{sf}^* = 0.1 and 0.5, significant thermal diode effect is shown, especially for low temperatures, i.e., $R_{max} \sim 6$ (Figure 2).
- The stronger solid-gas interaction surface (bottom surface) results in more adsorbed gas particles even when it has higher temperature compared to the weak surface (Figure 5)

Results and Discussions: Adsorption Isotherm

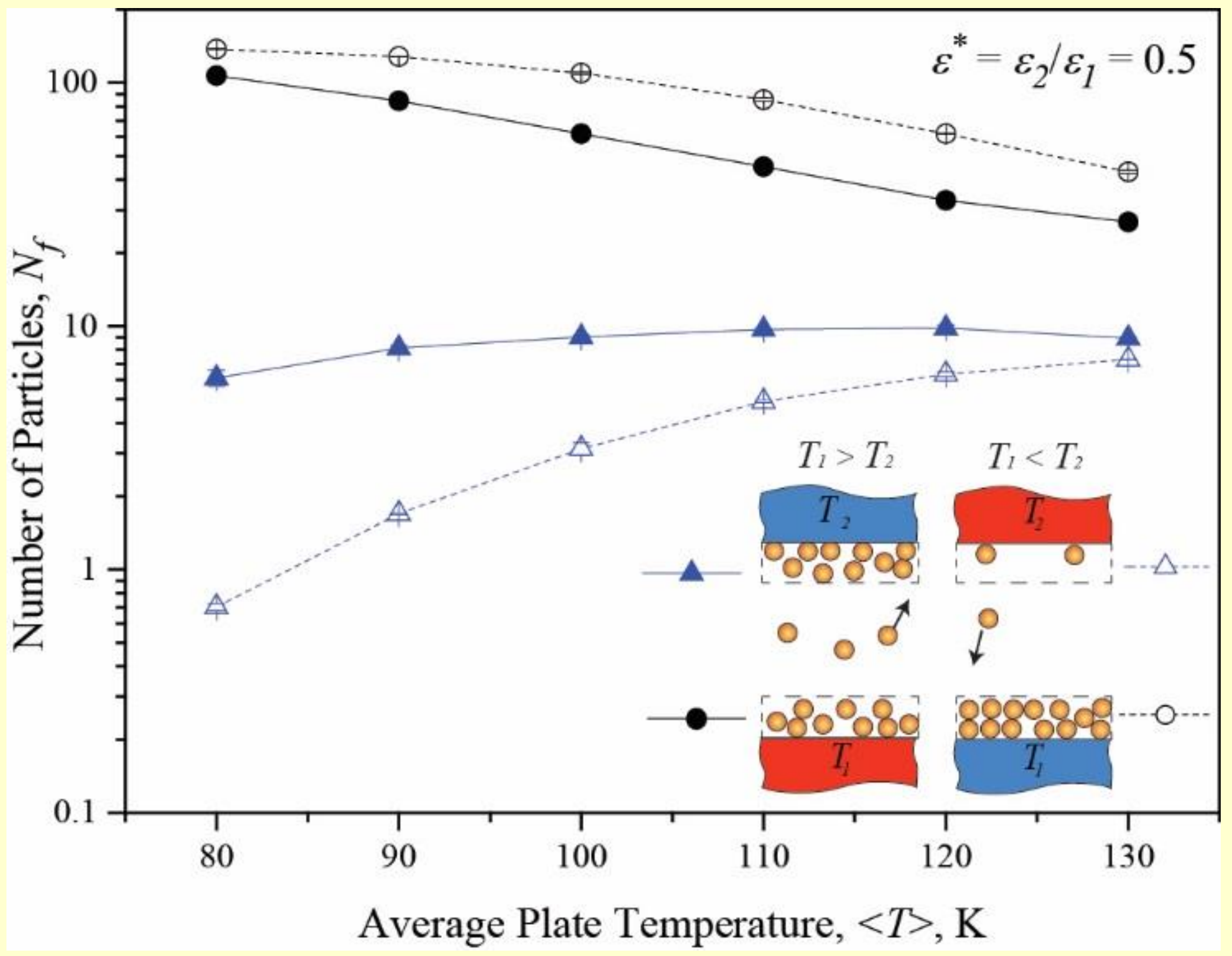


Figure 5. Distribution of the particles through the nanogap, ε^* = 0.5

Conclusion

- In this study, the adsorption-controlled thermal diode is examined using Ar gas-filled nanogap with heterogeneous solid-gas interactions.
- A maximum degree of rectification, $R_{max} \sim 10$, is found at T = 80 K which results from the significant adsorption-controlled thermal accommodation coefficient (TAC).
- The predicted results using the modeled surfaces (ε^* = 0.5 and 0.1) can be achievable using real materials. For instance, a ε^* = 0.5 represents Pb as the weak, and Pt as the strong surface to construct the nanogap.

Acknowledgment

This material is based upon work supported by the National Science Foundation under Award No. EPS-0903806 and matching support from the State of Kansas through the Kansas Board of Regents. This work is also partially supported by the start-up fund from the College of Engineering, Wichita State University. This work also used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575.

References

- Avanessian, T. and G. Hwang. *Adsorption-Based Thermal Rectifier*. in *ASME 2015 13th International Conference on Nanochannels, Microchannels, and Minichannels*. American Society of Mechanical Engineers.
- Hwang, G.S. & Kaviany, M. Molecular Dynamics Simulation of Effective Thermal Conductivity of Vapor-Filled Nanogap and Nanocavity. *Journal of Applied Physics* **106**, 024317 (2009).
- Maruyama, S. and T. Kimura, *A study on thermal resistance over a solid-liquid interface by the molecular dynamics method*. Therm. Sci. Eng, 1999. **7**(1): p. 63-68.