Thermal Transport in Various 1D Sturctures

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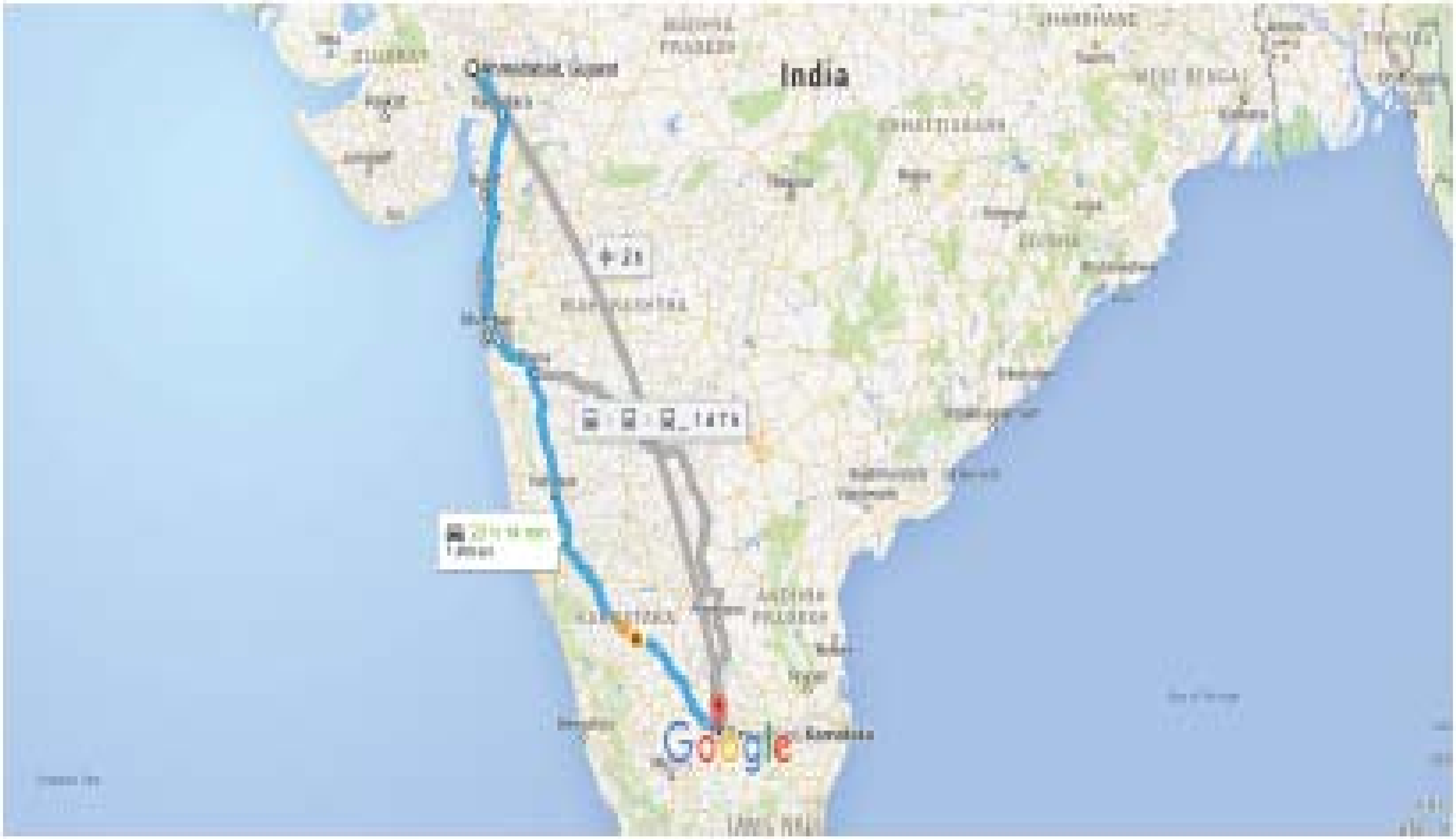
Google Maps Ahmedabad, Gujarat to Bangalore, Karnataka

Drive 1,495 km, 22 h 14 min



Map data ©2015 Google 200 km

Acknowledgements

- My Research Group
- Gujarat University, Ahmedabad, India

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- DRS-SAP-I, University Grants Commission, New Delhi, India

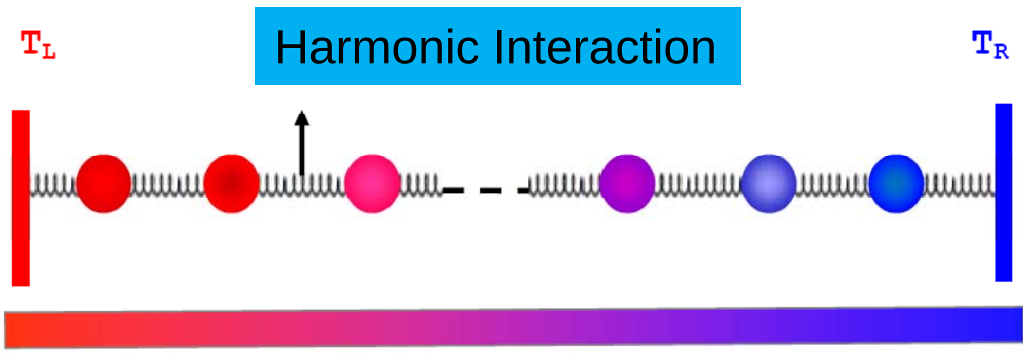
- Prof. Abhishek Dhar & ICTS, Bangalore

Thermal Transport in various 1D Structures:
Results of Our Simulations

- Linear Mass Graded Chain (Yang et al, 2007, P. N. Gajjar et al, 2010)
- Exponential Mass Graded Chain. (Tejal N. Shah & P.N. Gajjar, 2012)
- Diatomic Chain (Tejal N. Shah & P. N. Gajjar, 2012)
- Mass Defective Chain (Tejal N. Shah & P. N. Gajjar, 2012)
- Abrupt Junction Thermal Diode (P. P. Patel & P. N. Gajjar, 2013)
- Composite Materials (P. P. Patel & P. N. Gajjar, 2013)
- Sandwitch Structure (Tarika K. Patel & P. N. Gajjar, 2015)
- Tri-Mass Segment Thermal Transistor (P. P. Patel & P. N. Gajjar, 2013)
- Characteristics of Thermal Transistor (M.G.Vachhani & P.N.Gajjar, 2015)

Heat conduction in 1-D Chain:

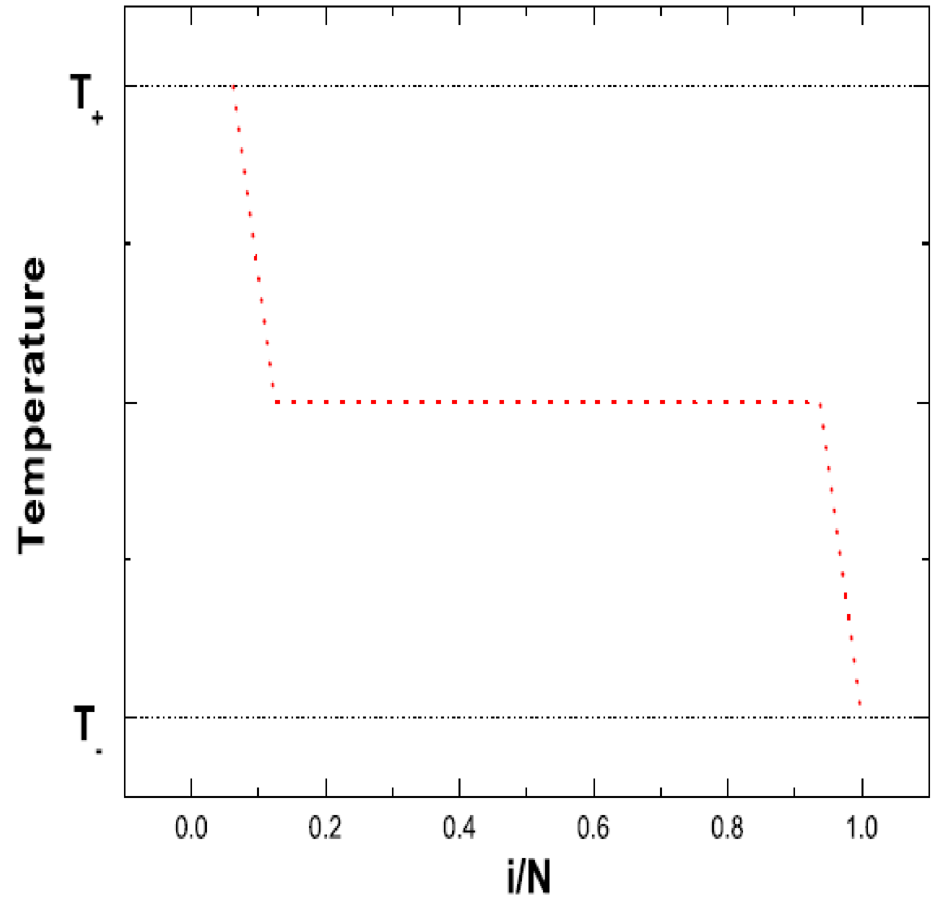
Harmonic



$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + \frac{1}{2}(x_i - x_{i+1})^2 \right]$$

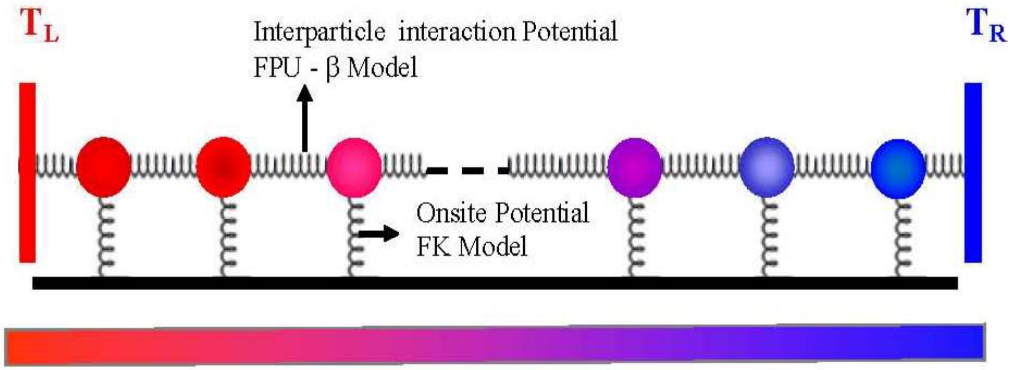
$$J = -\kappa \nabla T$$

Broken of Fourier's law

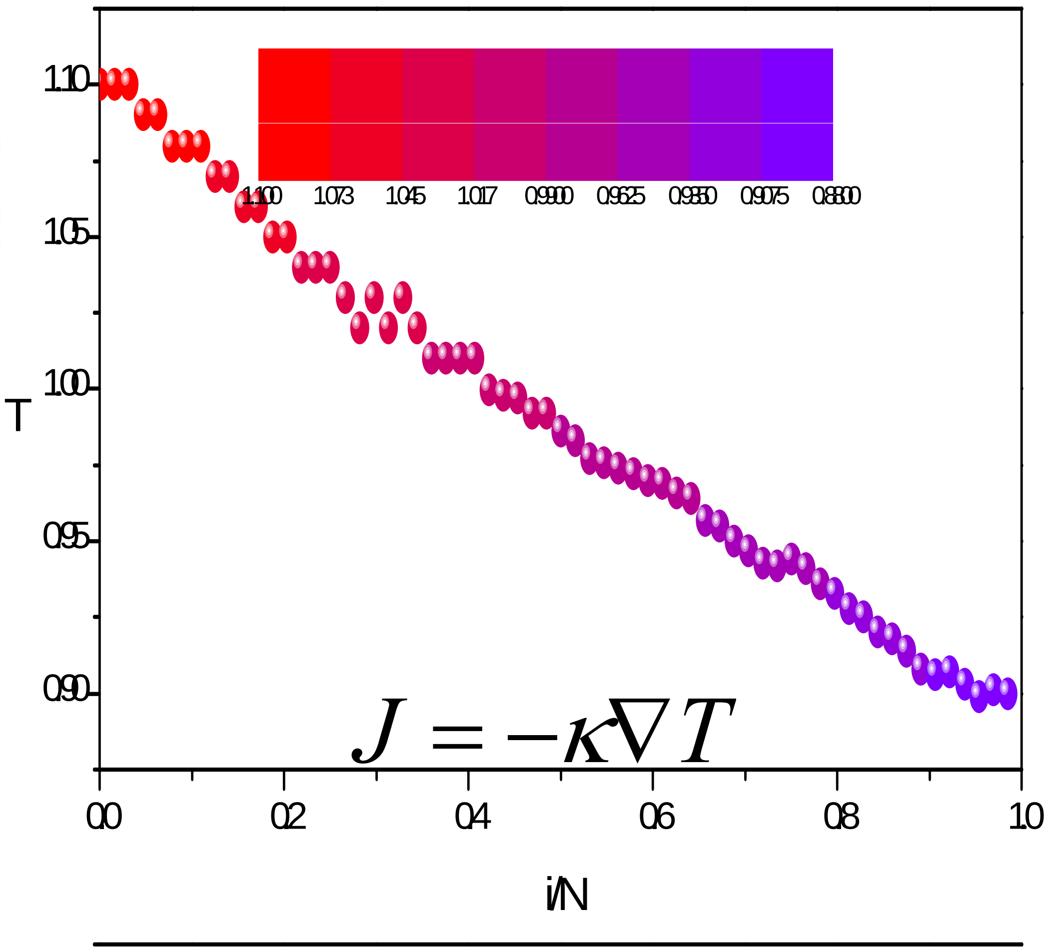


Heat conduction in 1-D Chain:

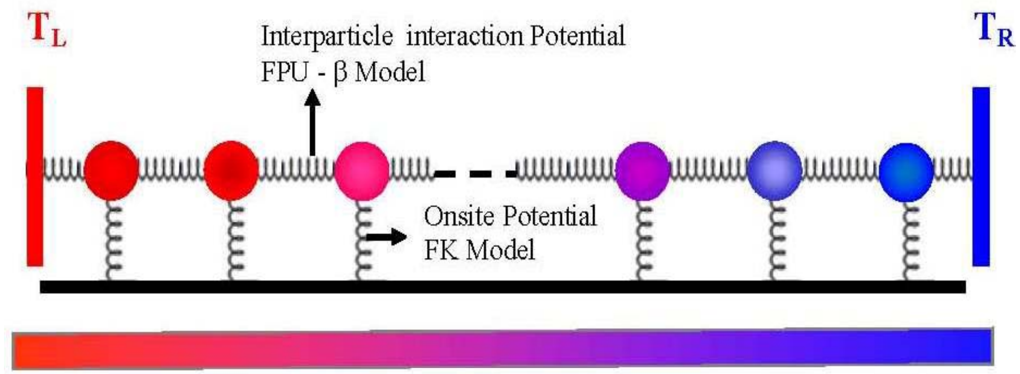
Anharmonic (Tejal N. Shah & P. N. Gajjar, 2012, 2013)

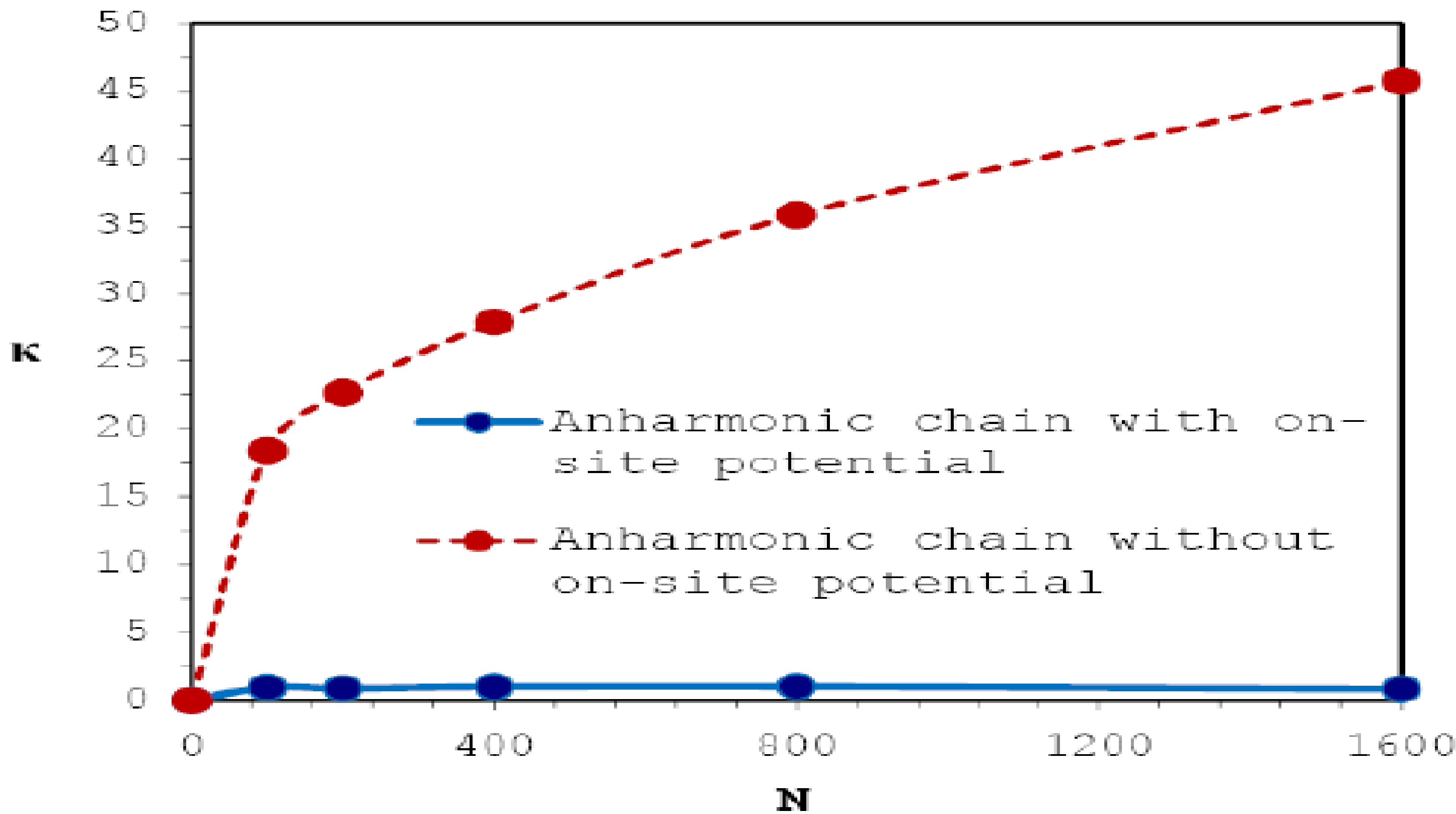


$$H_i = \frac{p_i^2}{2} + V(x_{i-1}, x_i) + U(x_i).$$



Thermal Conductivity





Controversy over the critical exponent α

For anomalous heat conduction, some of the predicted values of α are:

(i) $\alpha = 1$ for harmonic lattices

(ii) $\alpha = 0.5$ for disordered harmonic lattices

(iii) $0 < \alpha < 1$ for FK lattices

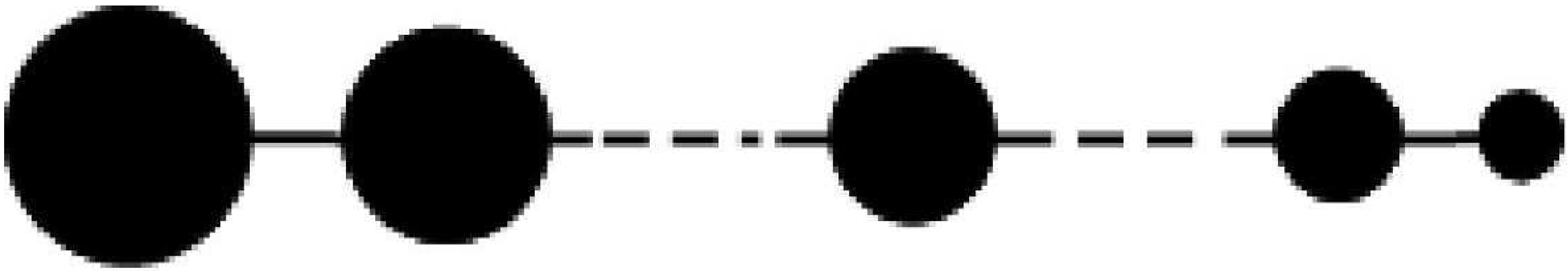
(iv) $0.34 < \alpha < 0.44$ for FPU lattices

(v) $0.22 < \alpha < 0.35$ for hard sphere model

(vi) $\alpha = 0.22$ for triangular model

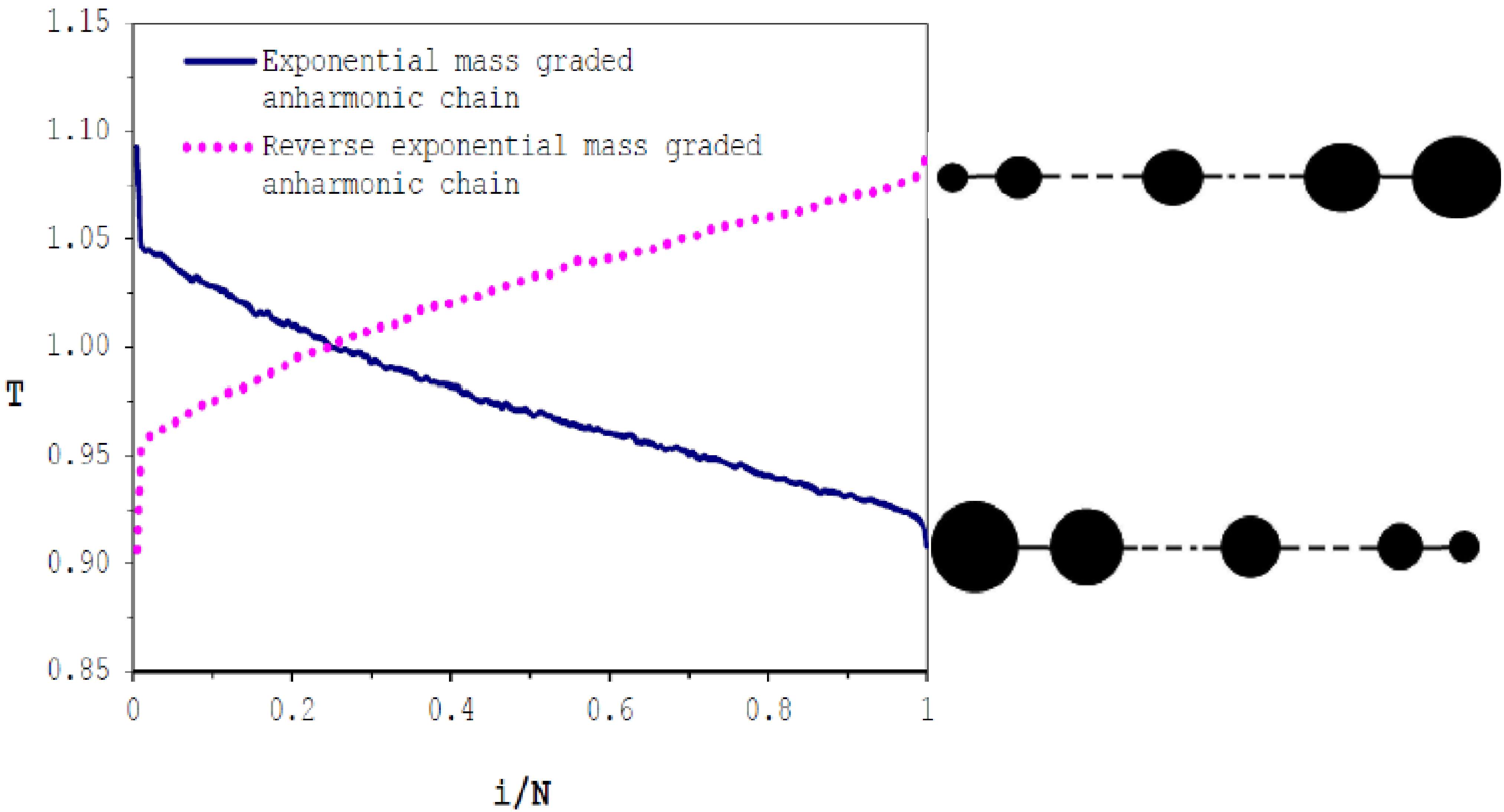
Etc…….

Functional Materials:
Thermal Rectification and NDTR



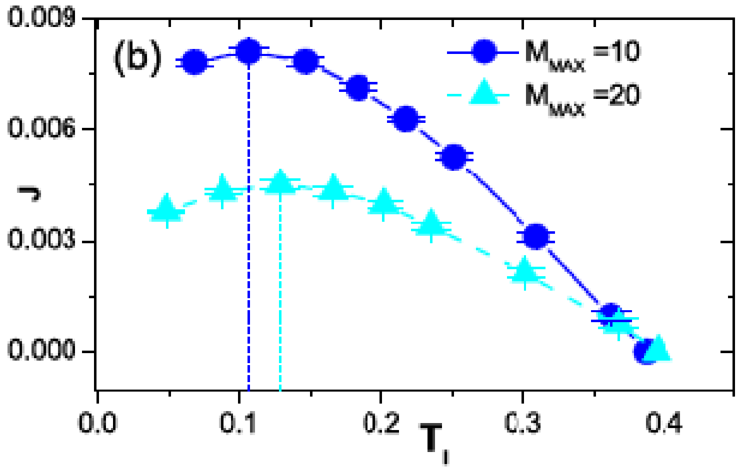
- Linear Mass graded Chain.
- Exponential Mass graded Chain.

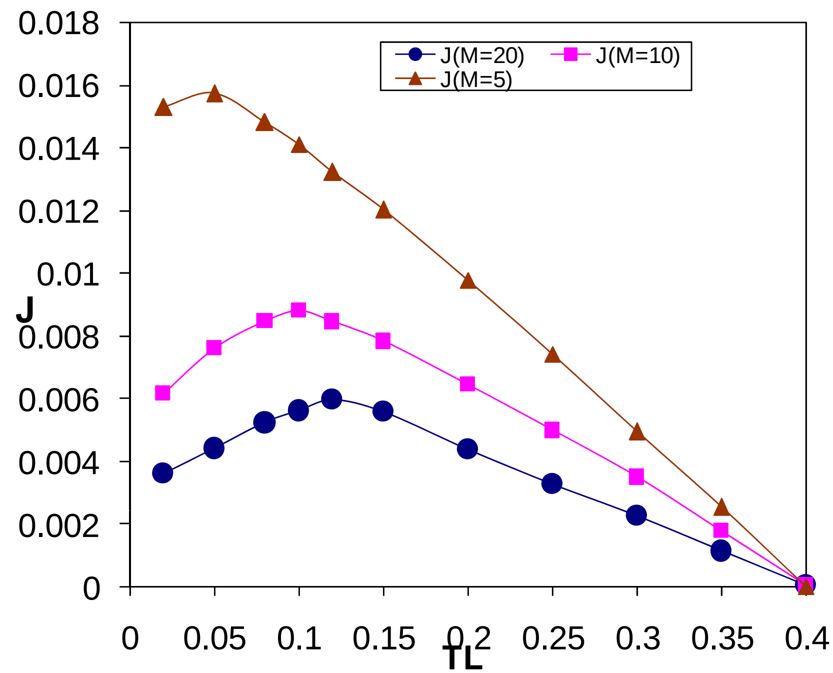
Temperature Profiles



Linear Vs Exponential Mass Graded Chains

Yang et al, 2007

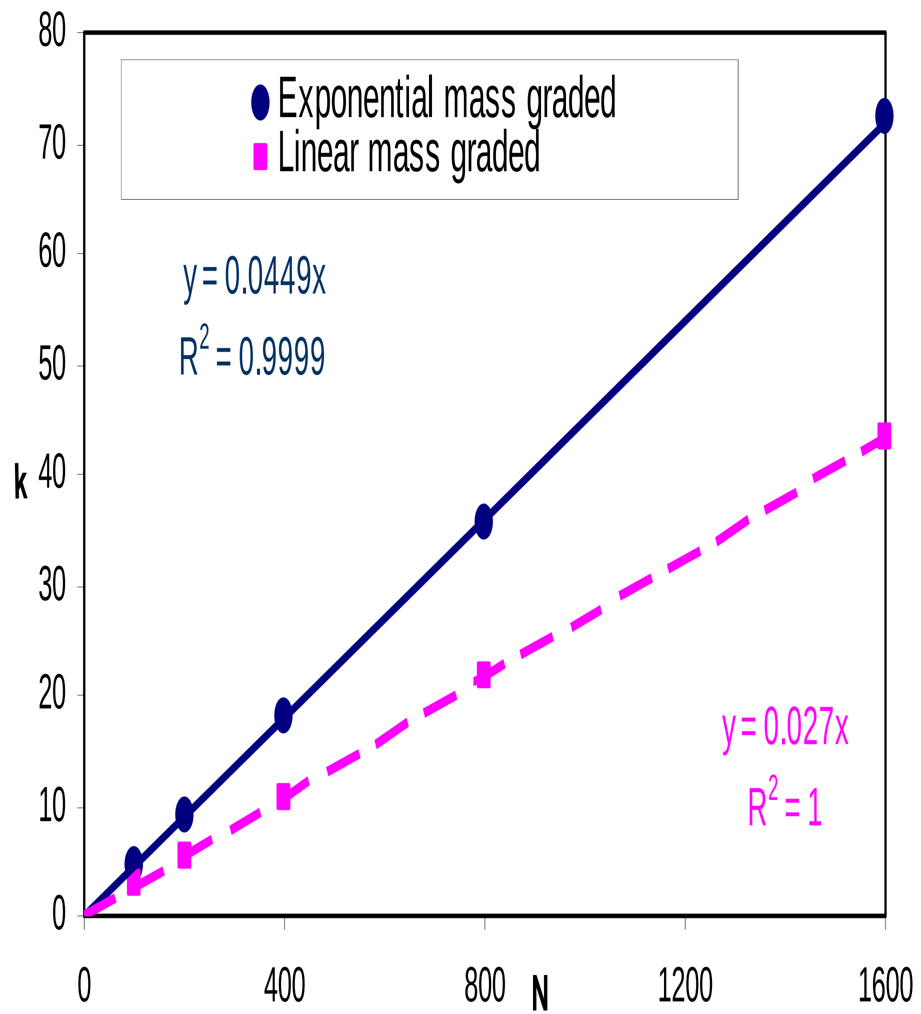




- **Important feature in 1-D graded chain → Negative Differential Thermal Resistance.**

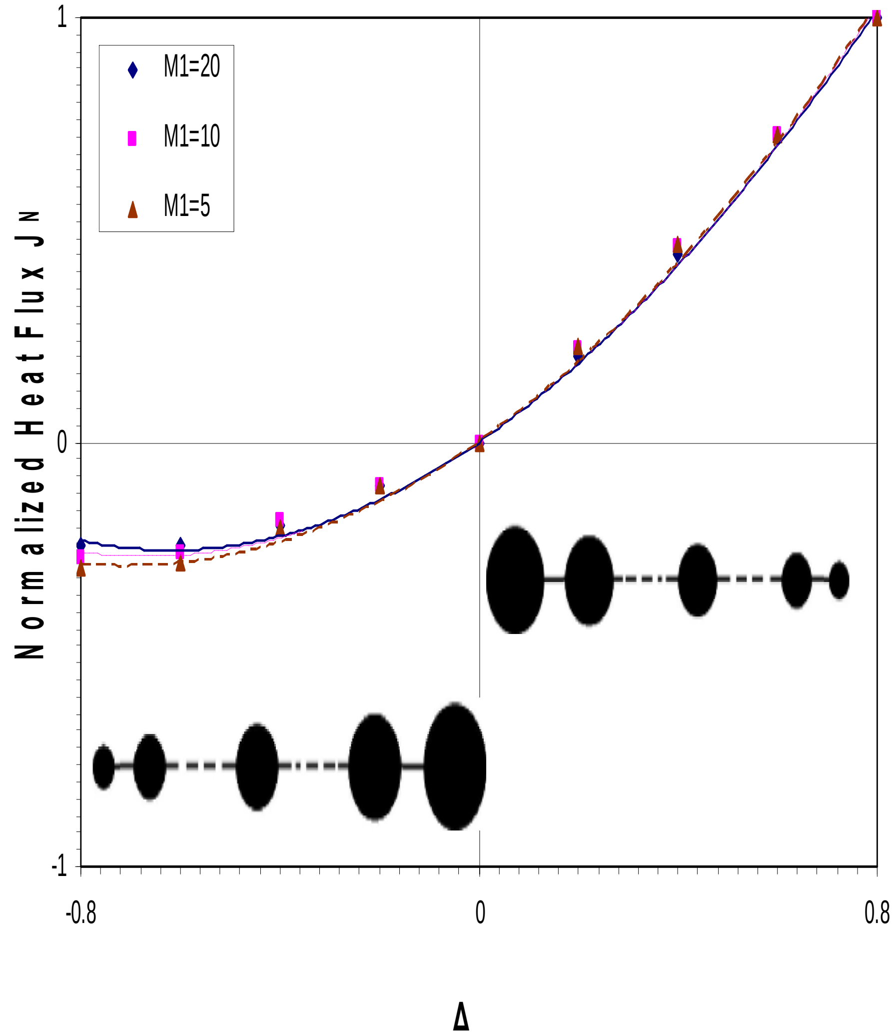
Linear Vs Exponential Mass Graded Chains

- **Exponential Mass graded chain Ƙ = 0.045 N**
- **Linear Mass graded chain of Yang et al. is Ƙ = 0.027 N.**
- **Thus compared to linear mass graded harmonic lattice, the exponential mass graded harmonic lattice works as a better thermal conductor.**
- **(Tejal N Shah & P. N. Gajjar: Physics Letters A 376, 438 (2012))**

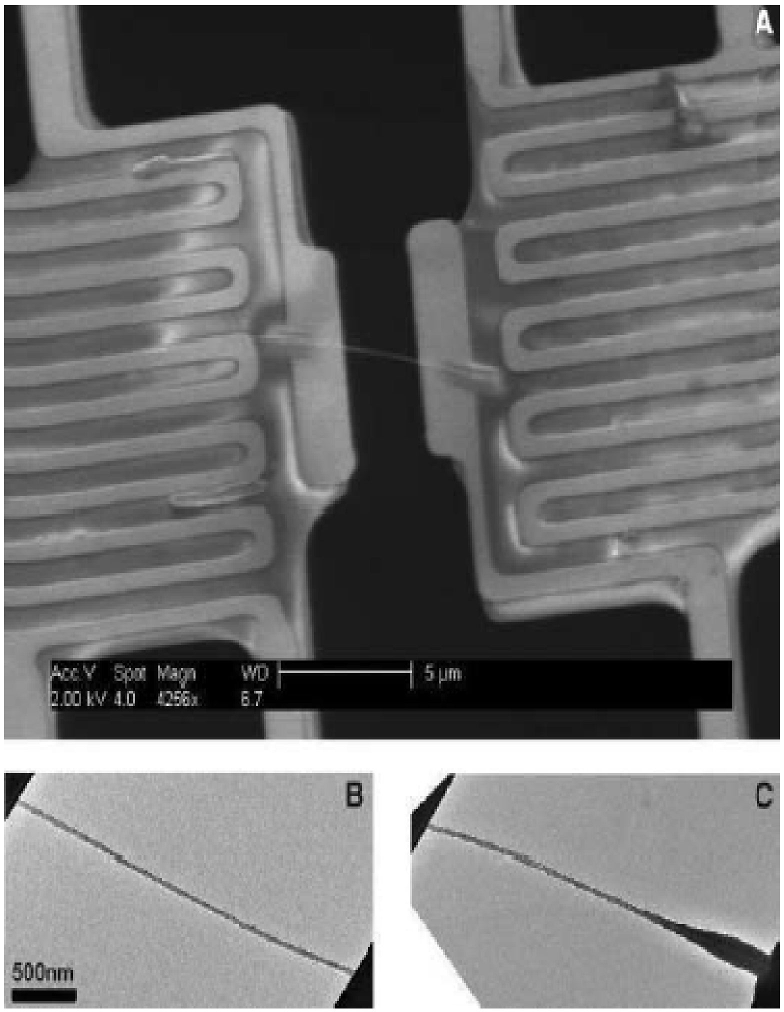


- We have also studied the thermal rectification in the exponential mass graded anharmonic lattice.

- The present model of exponential mass graded anharmonic chain generates the thermal rectification of 70-75%.



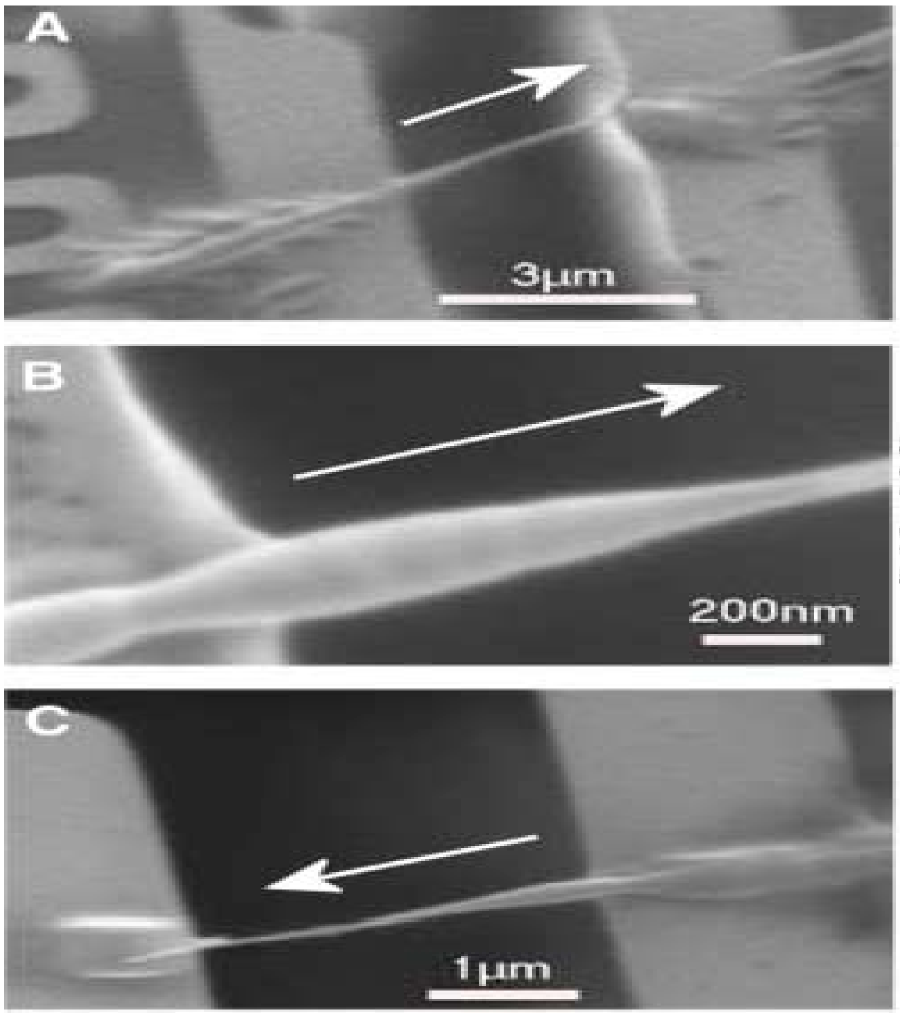
First Solid State Thermal Rectifier

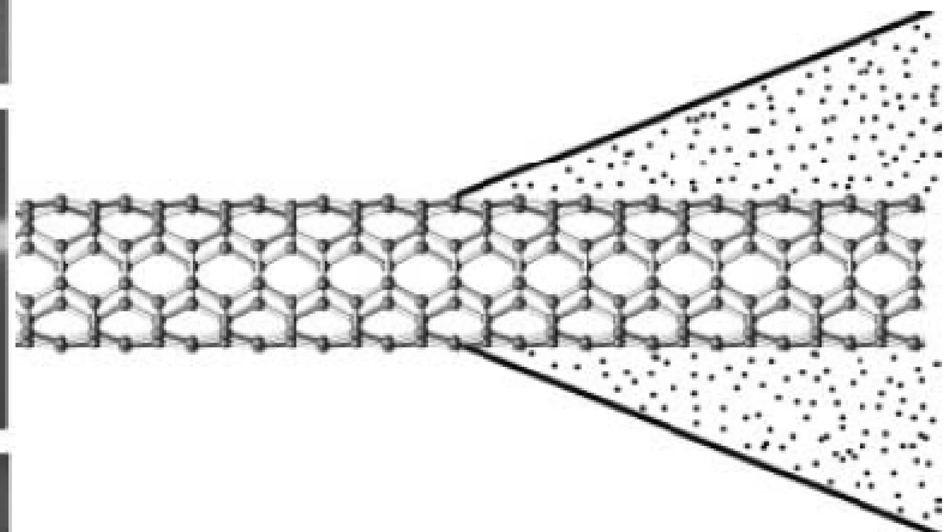


Chang et al. built the first microscopic solid state thermal diode. They attached a heater and a sensor to the two ends of a carbon nanotube and calculated its thermal conductivity. Then they deposited amorphous $C_9H_{16}Pt$ non-uniformly along the half length of the nanotube to vary the temperature dependence of the resonance frequency along the nanotube and achieved conductance of 3-7% greater in one direction than it was in the other.

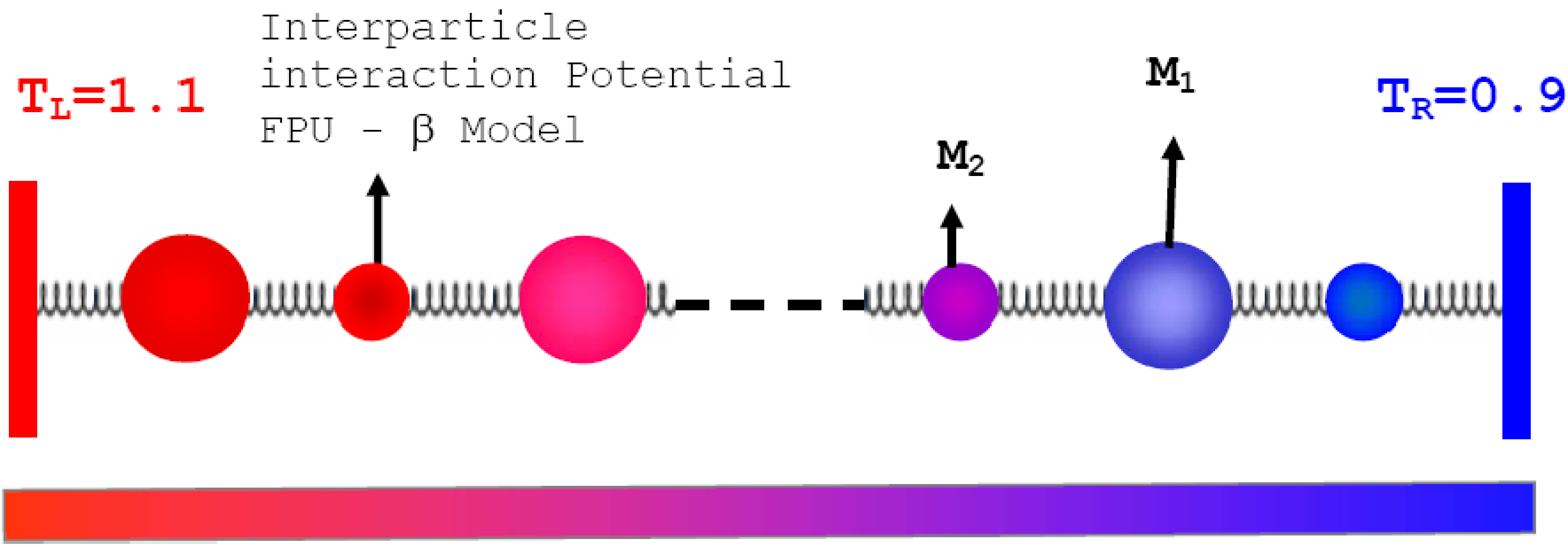
(C. Chang, D. Okawa, A. Majumdar and A. Zettl, Science 314 (2006)121.)

First Solid State Thermal Rectifier

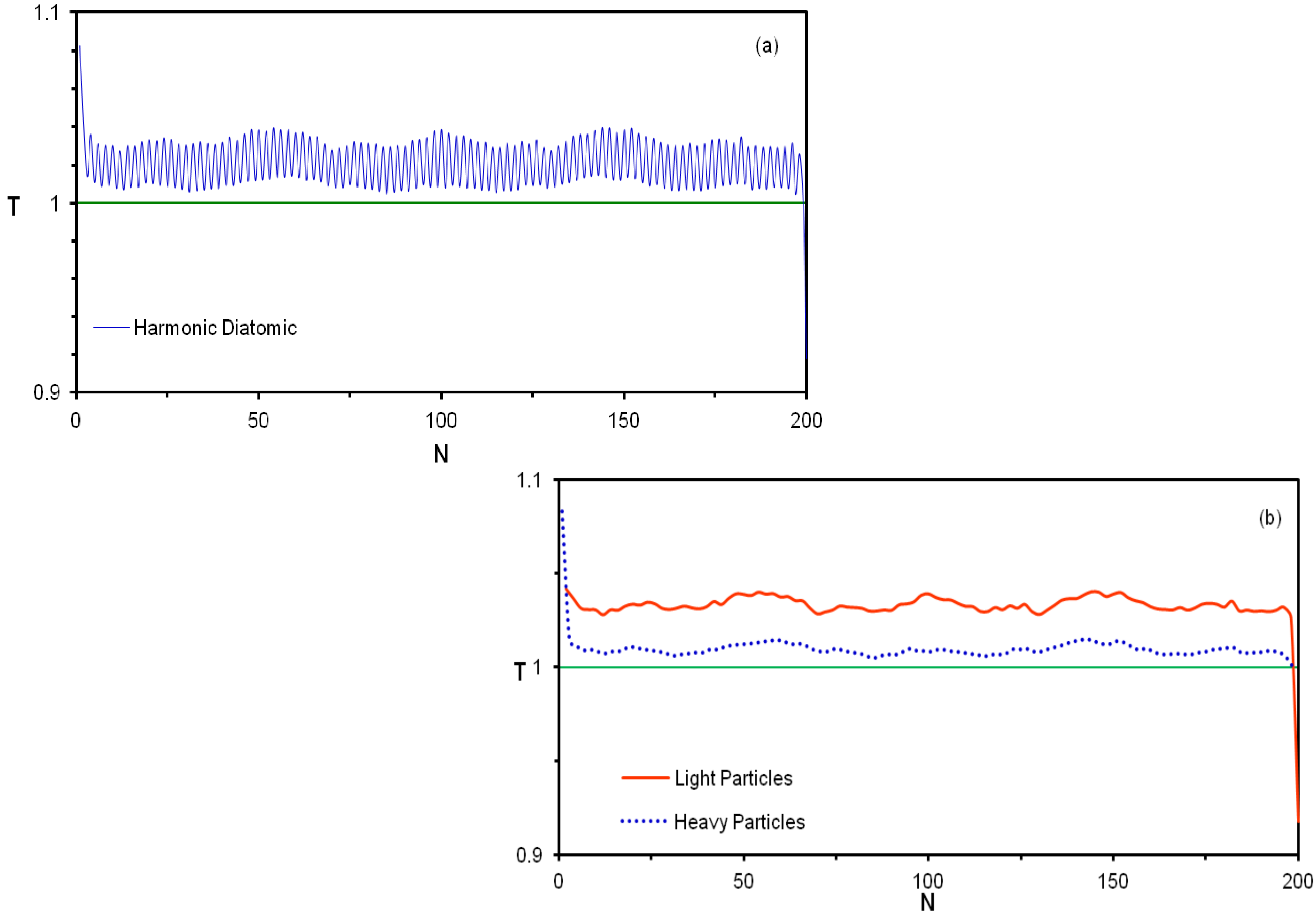




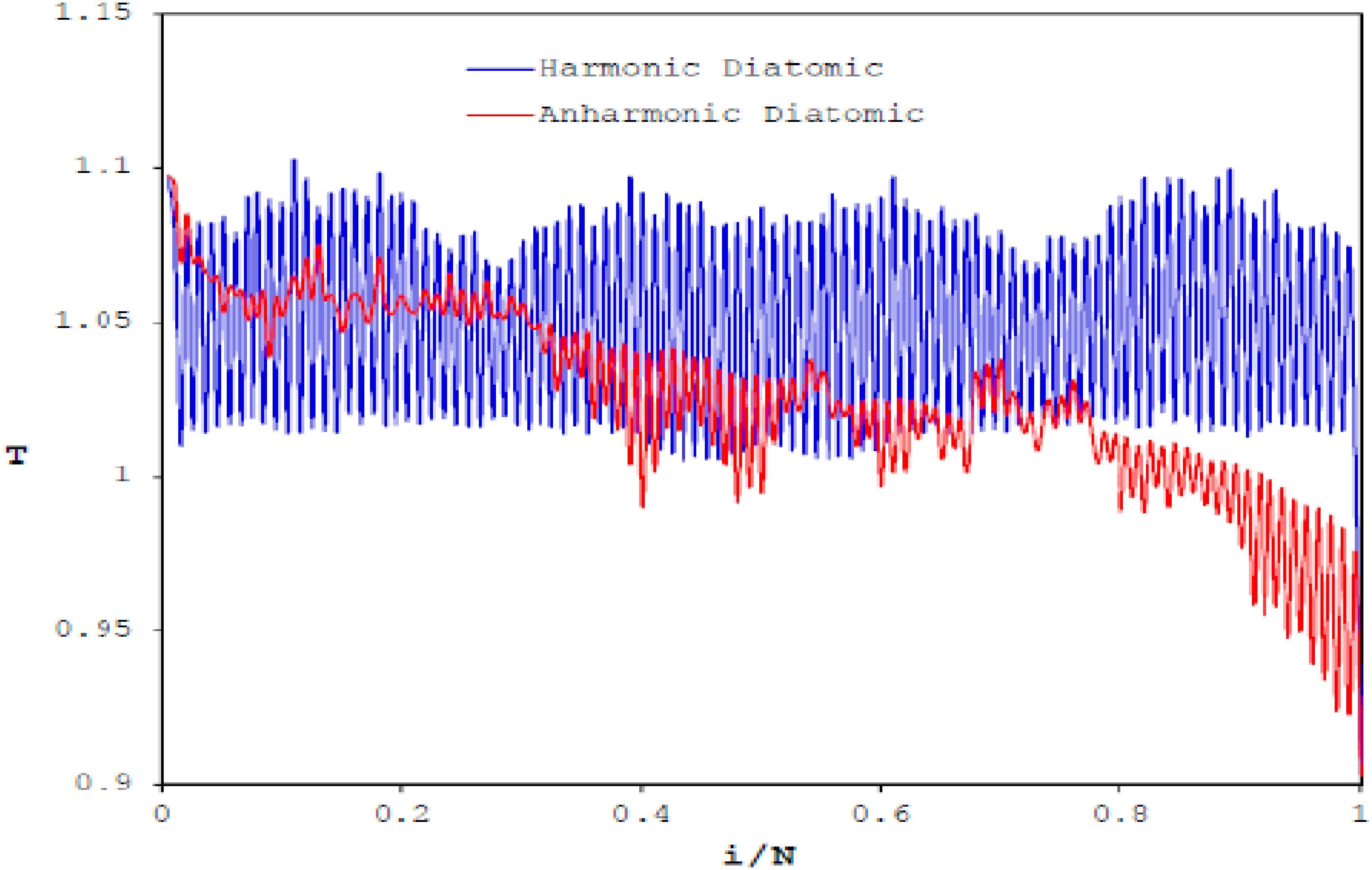
Diatomic Chain
Tejal N. Shah & P. N. Gajjar, 2012



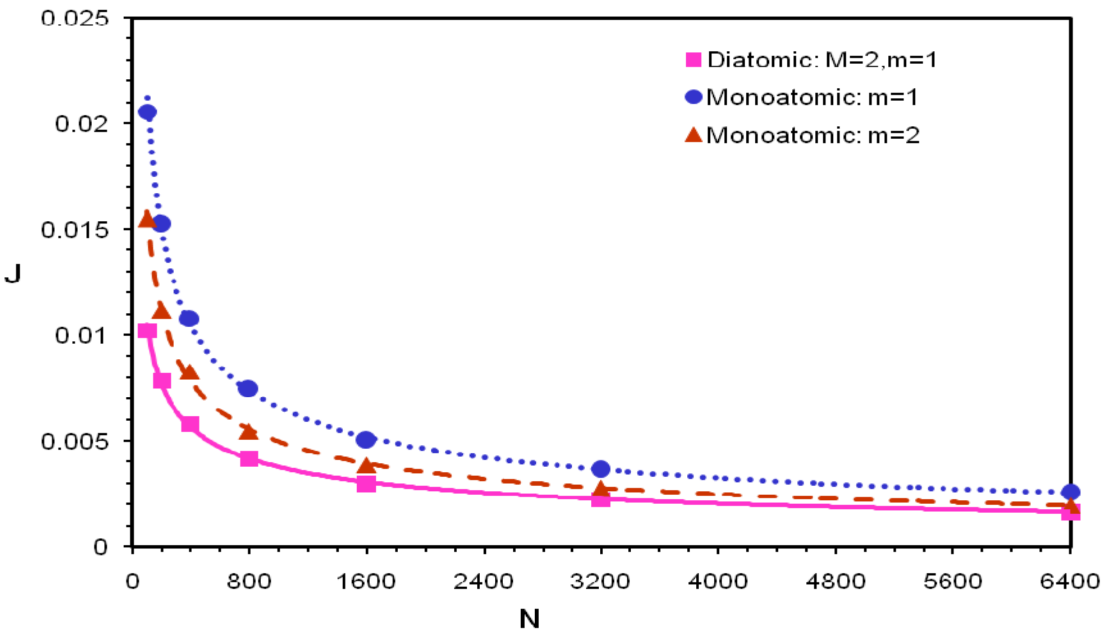
Tejal N. Shah & P. N. Gajjar, 2012

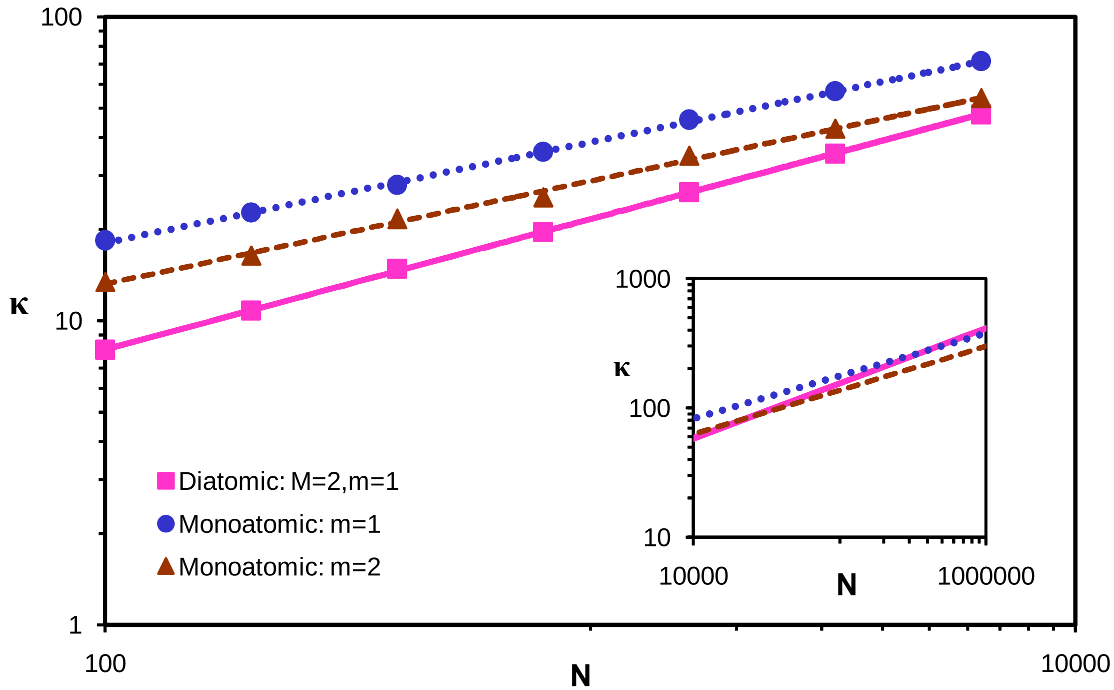


(a)
Harmonic Diatomic
T
1.1
1
0.9
0
50
100
150
200
N
(b)
Light Particles
Heavy Particles
T
1.1
1
0.9
0
50
100
150
200
N

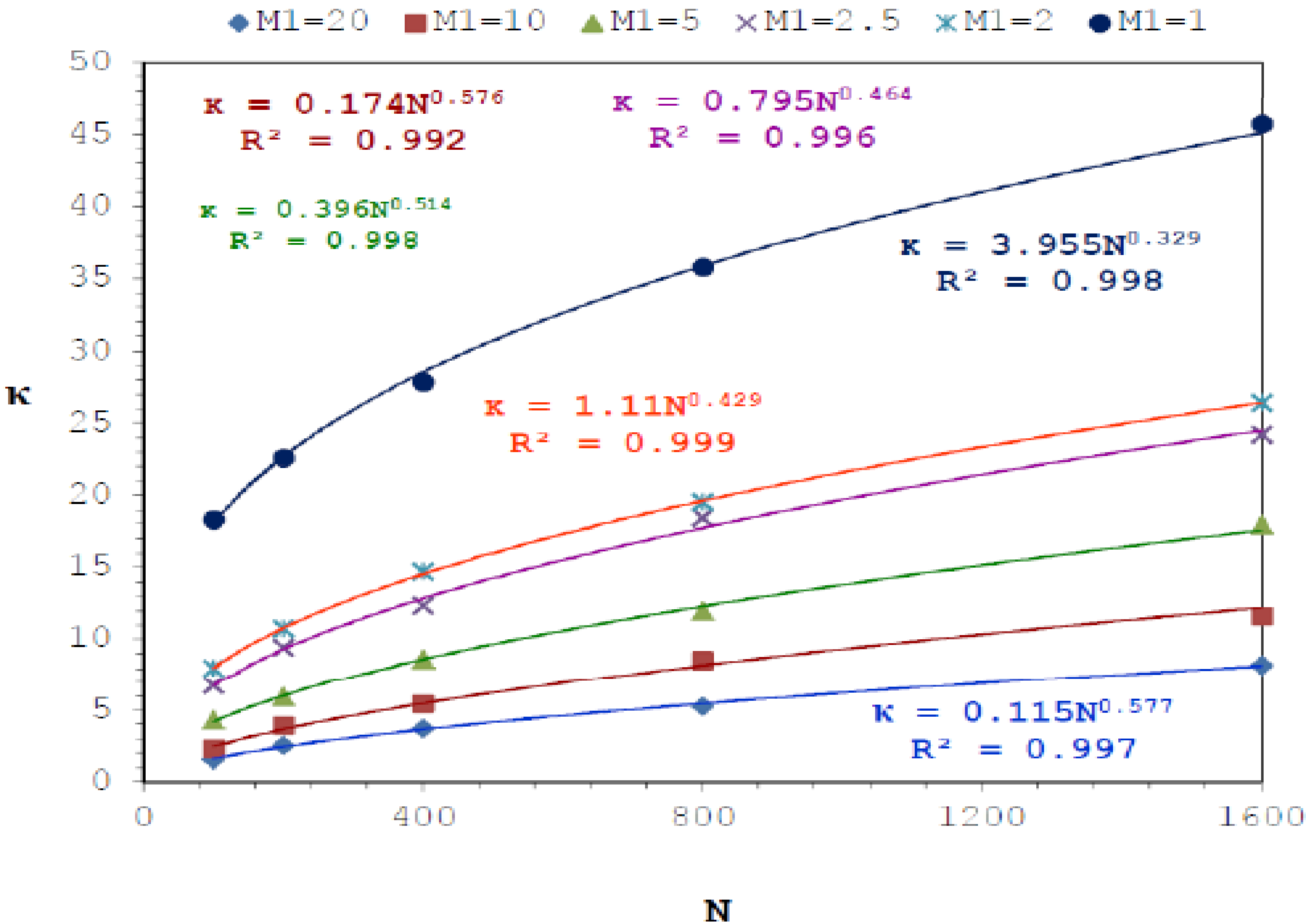


Harmonic Diatomic
Anharmonic Diatomic
1.15
1.1
1.05
1
0.95
0.9
T
0
0.2
0.4
0.6
0.8
1
i/N

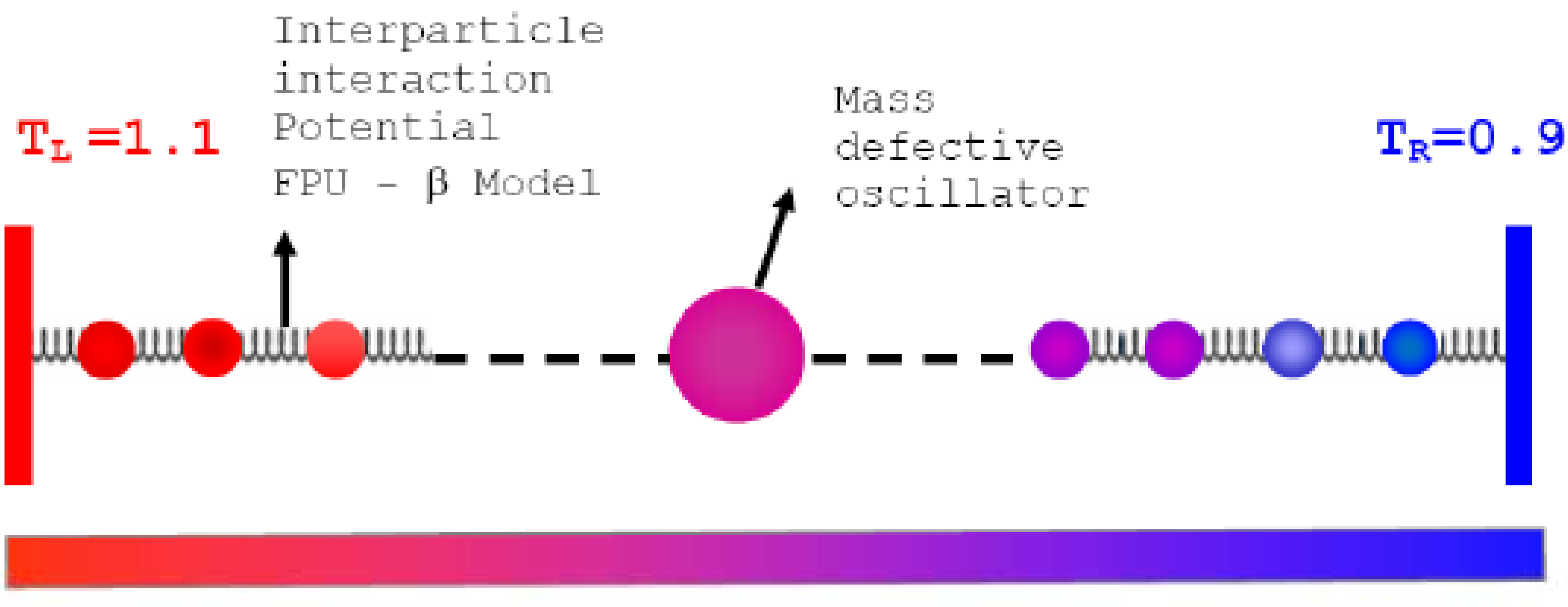




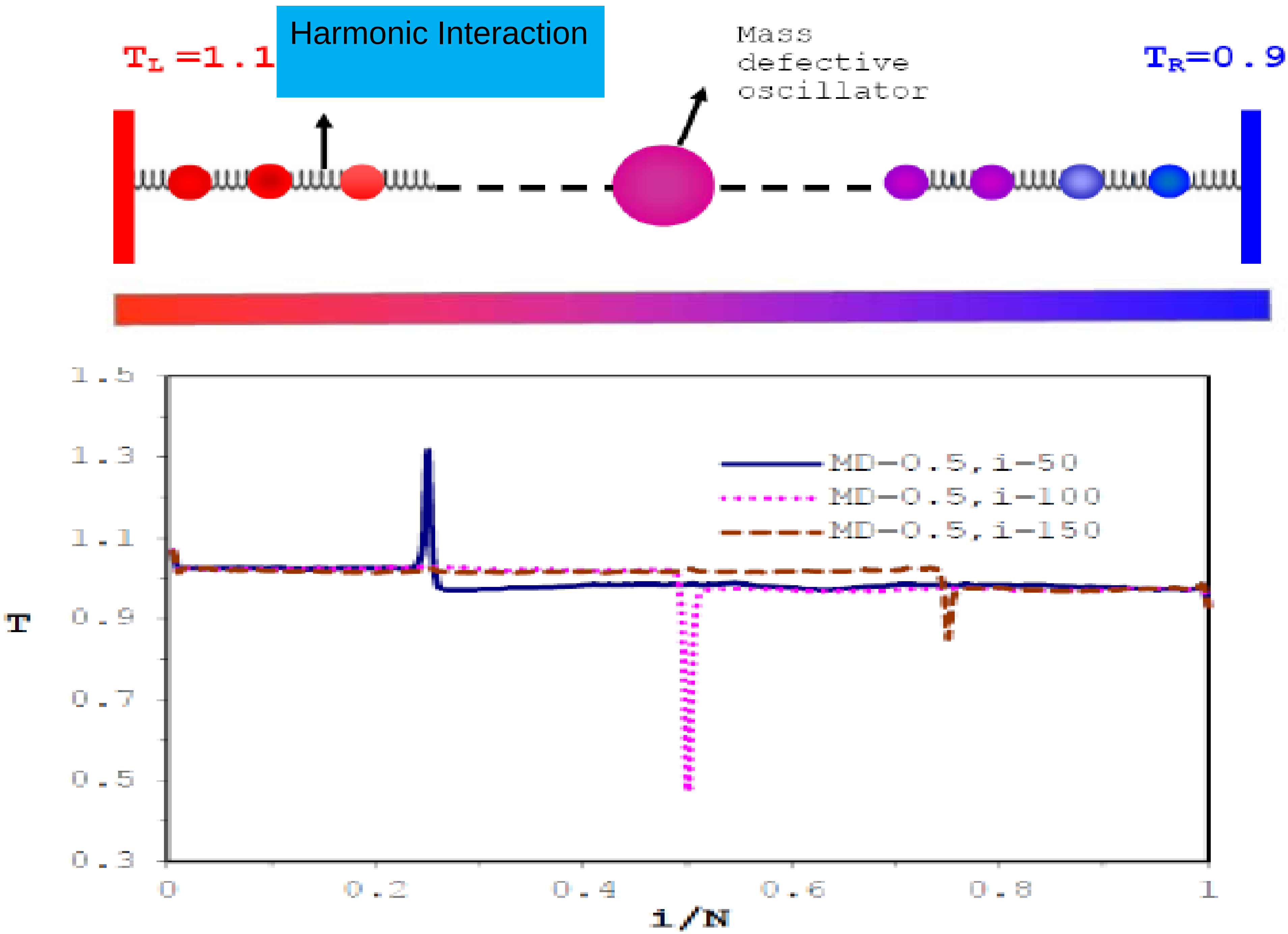
The power divergent exponent of thermal conductivity 0.428±0.001 and diffusion exponent 1.2723 lead to the conclusions that increase in the system size, increases the thermal conductivity and existence of anomalous energy diffusion.

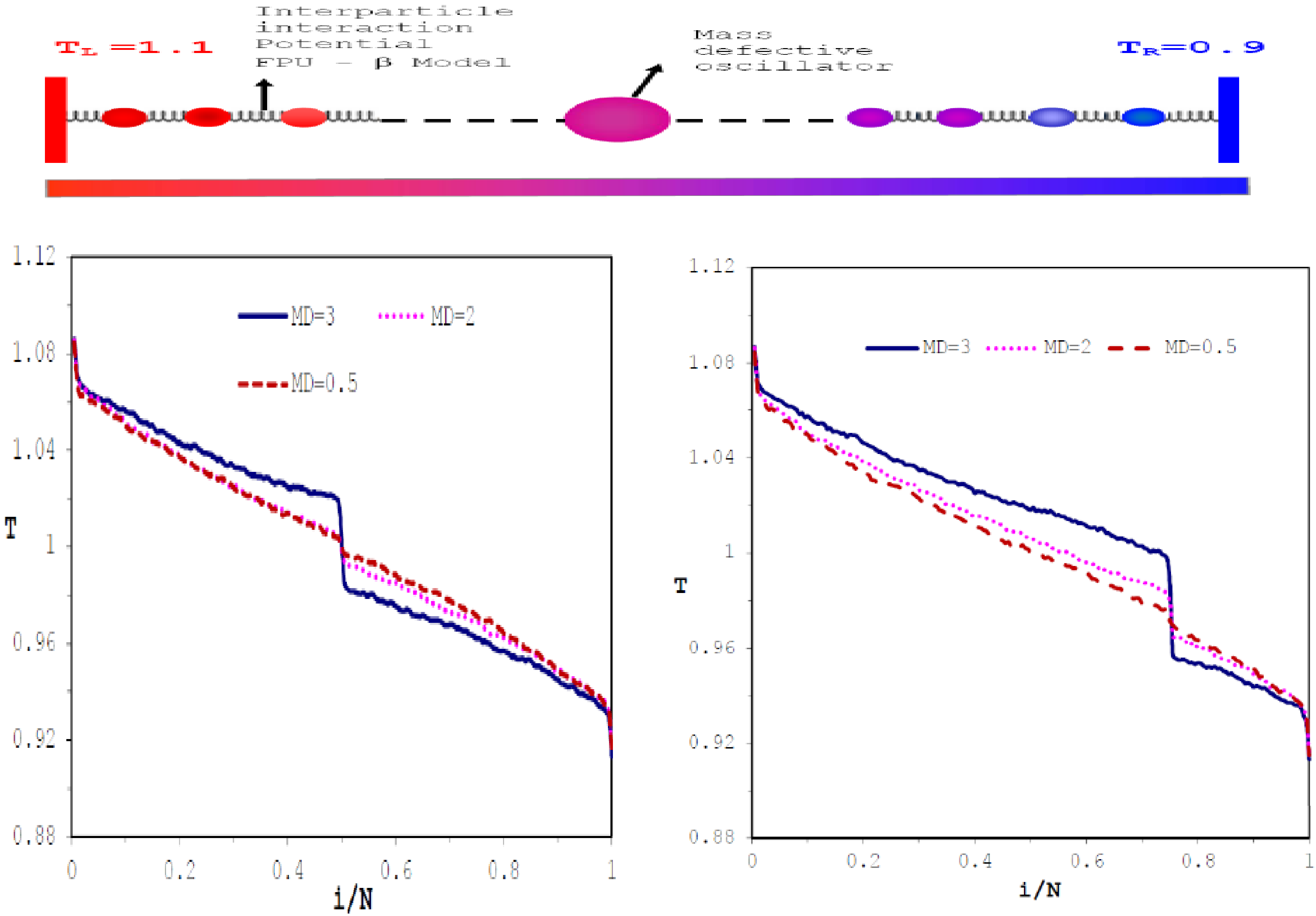

M1=20
M1=10
M1=5
M1=2.5
M1=2
M1=1
κ = 0.174N^0.576
R² = 0.992
κ = 0.795N^0.464
R² = 0.996
κ = 0.396N^0.514
R² = 0.998
κ = 3.955N^0.329
R² = 0.998
κ = 1.11N^0.429
R² = 0.999
κ = 0.115N^0.577
R² = 0.997
κ
N
0
5
10
15
20
25
30
35
40
45
50
0
400
800
1200
1600

Mass Defective Chain
Tejal N. Shah & P. N. Gajjar, 2012



Tejal N. Shah & P. N. Gajjar, 2012


Harmonic Interaction
T_L =1.1
Mass defective oscillator
T_R=0.9
MD-0.5,i-50
MD-0.5,i-100
MD-0.5,i-150
T
i/N
1.5
1.3
1.1
0.9
0.7
0.5
0.3
0
0.2
0.4
0.6
0.8
1

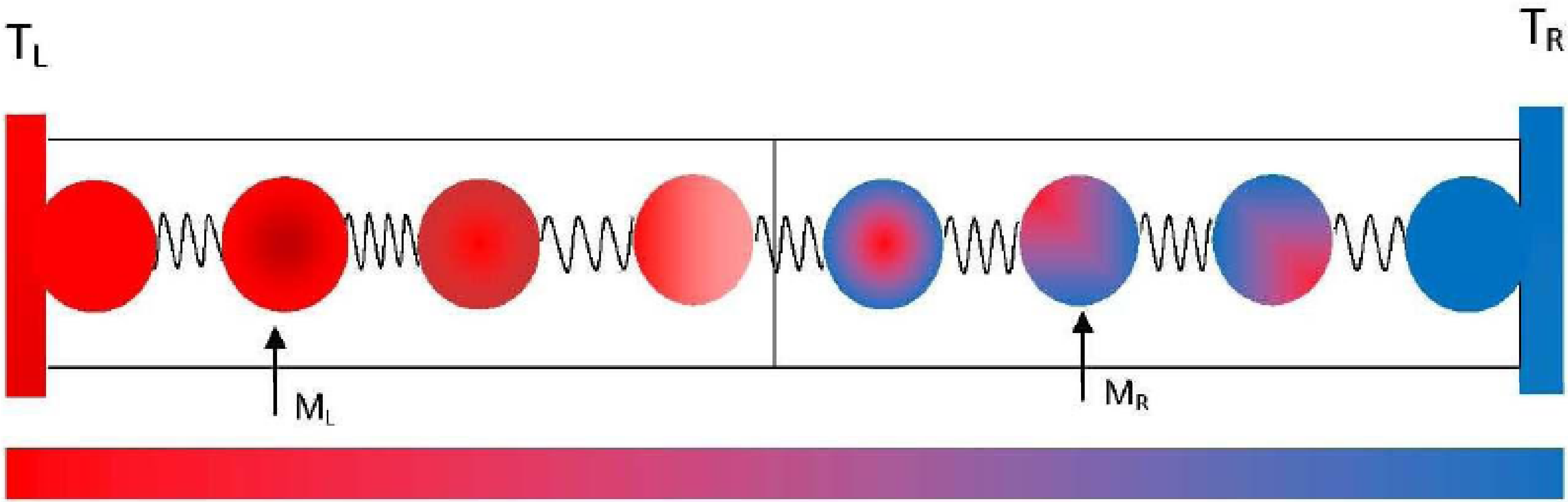


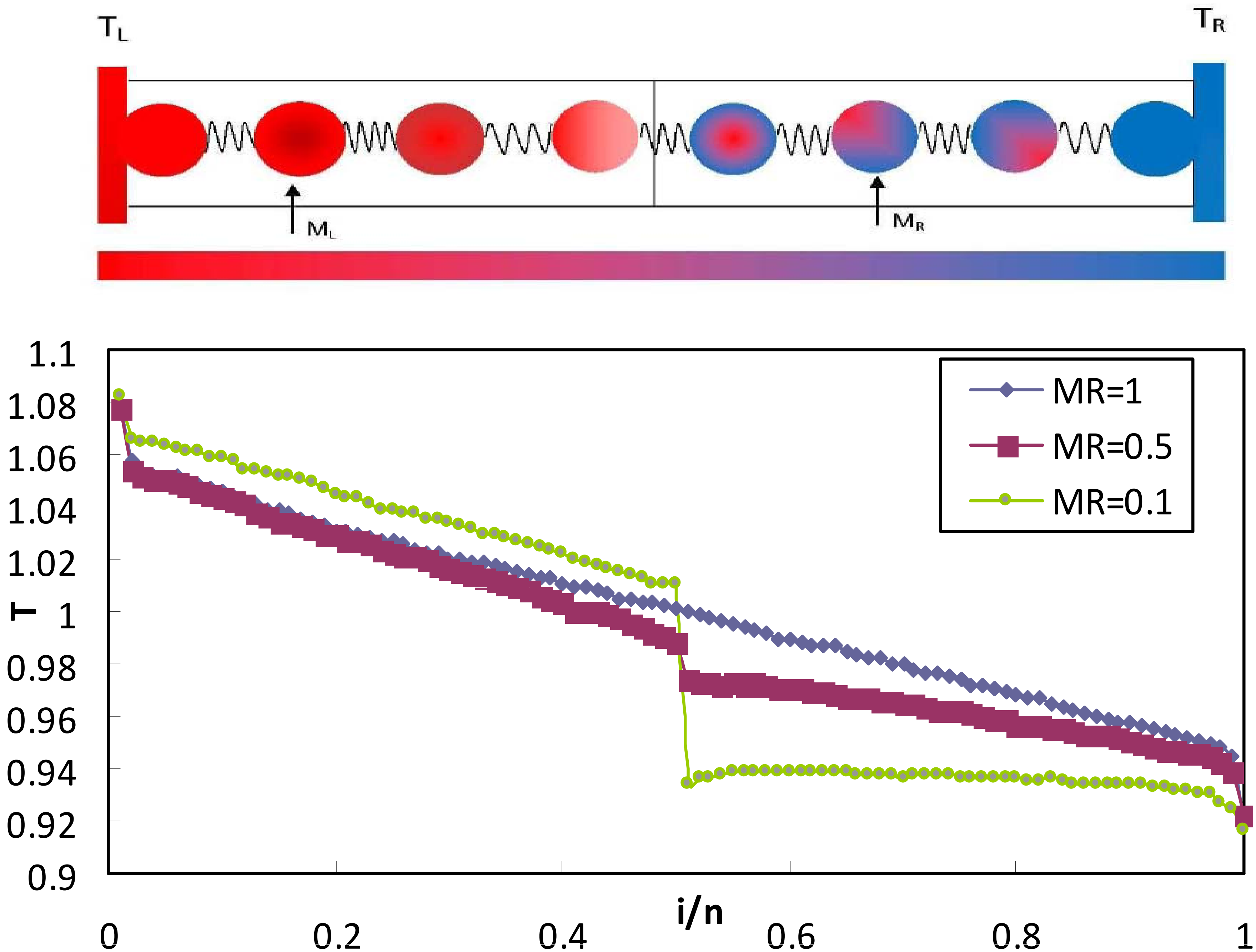
T_L =1.1
Interparticle
interaction
Potential
FPU – β Model
Mass
defective
oscillator
T_R=0.9
1.12
1.08
1.04
1
0.96
0.92
0.88
T
0
0.2
0.4
0.6
0.8
1
i/N
MD=3
MD=2
MD=0.5

Mass of the defected oscillator M_D	Defect Position i_D	Thermal conductivity κ
0.5	50	186.83
	100	176.75
	150	197.41
2.0	50	58.85
	100	58.75
	150	60.65
3.0	50	21.83
	100	22.93
	150	23.46

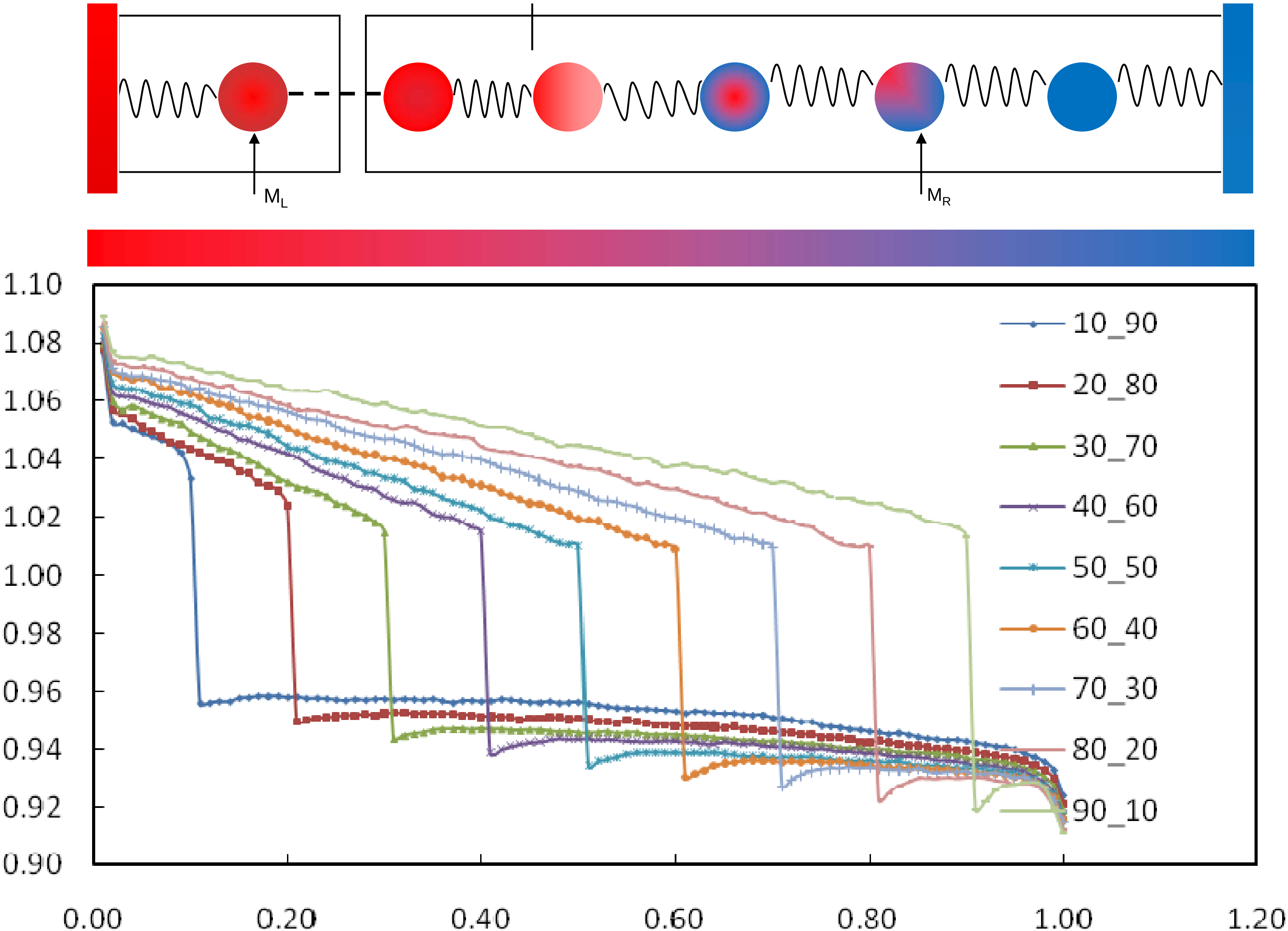
Abrupt Junction Thermal Diode

P. P. Patel & P. N. Gajjar, 2013

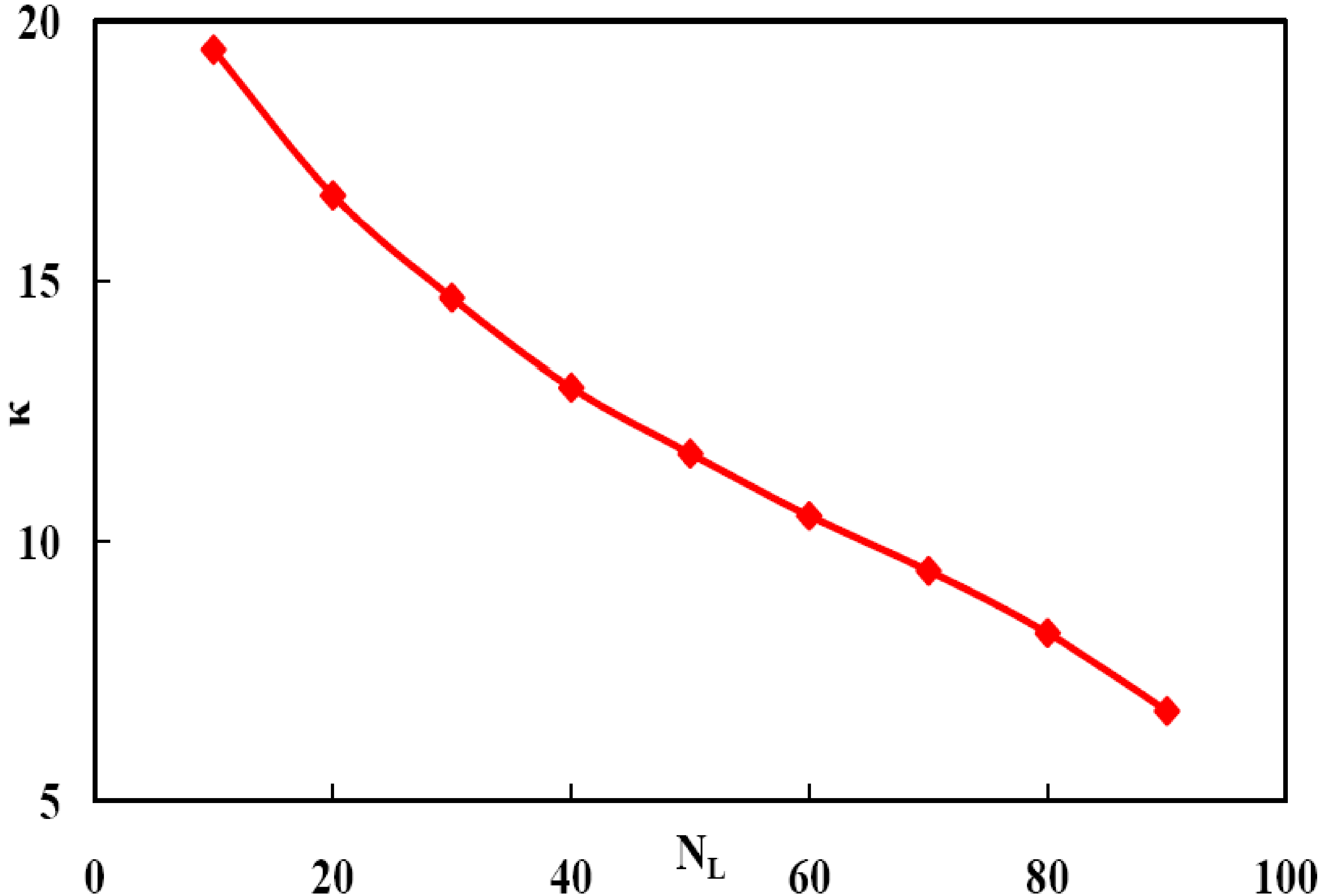




T_L
T_R
M_L
M_R
1.1
1.08
1.06
1.04
1.02
1
0.98
0.96
0.94
0.92
0.9
T
0
0.2
0.4
0.6
0.8
1
i/n
MR=1
MR=0.5
MR=0.1

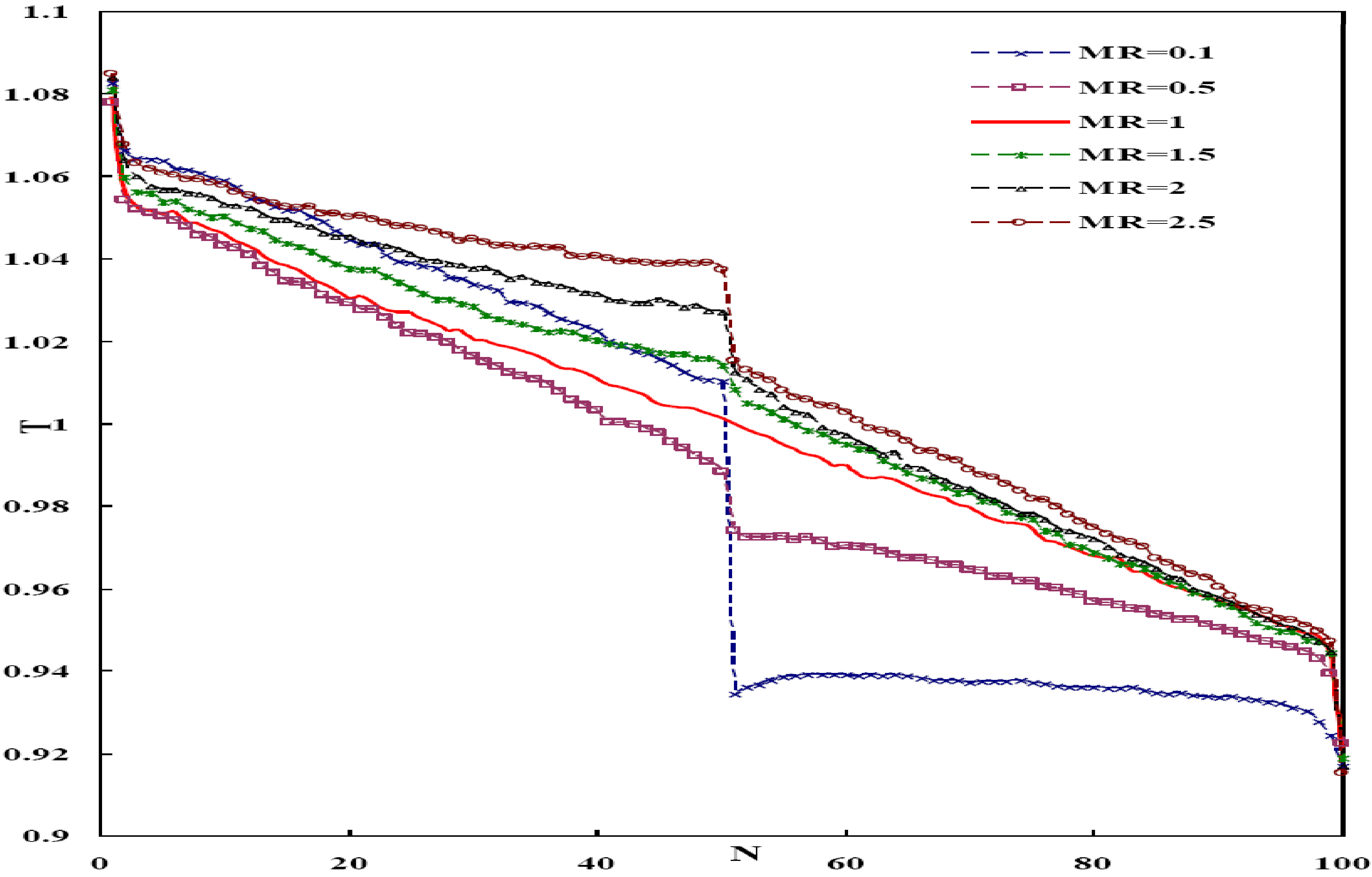


M_L
M_R
1.10
1.08
1.06
1.04
1.02
1.00
0.98
0.96
0.94
0.92
0.90
0.00
0.20
0.40
0.60
0.80
1.00
1.20
10_90
20_80
30_70
40_60
50_50
60_40
70_30
80_20
90_10

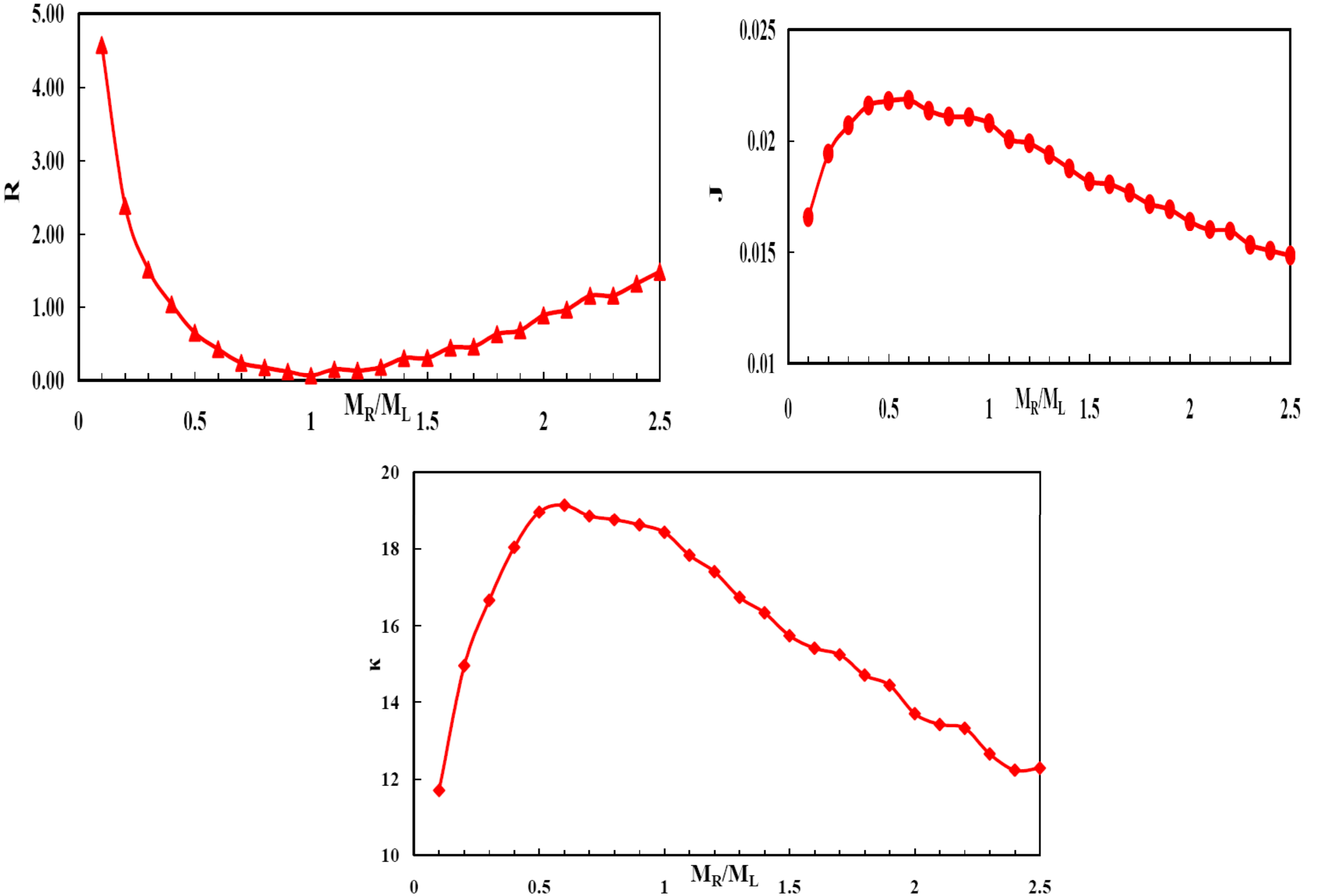


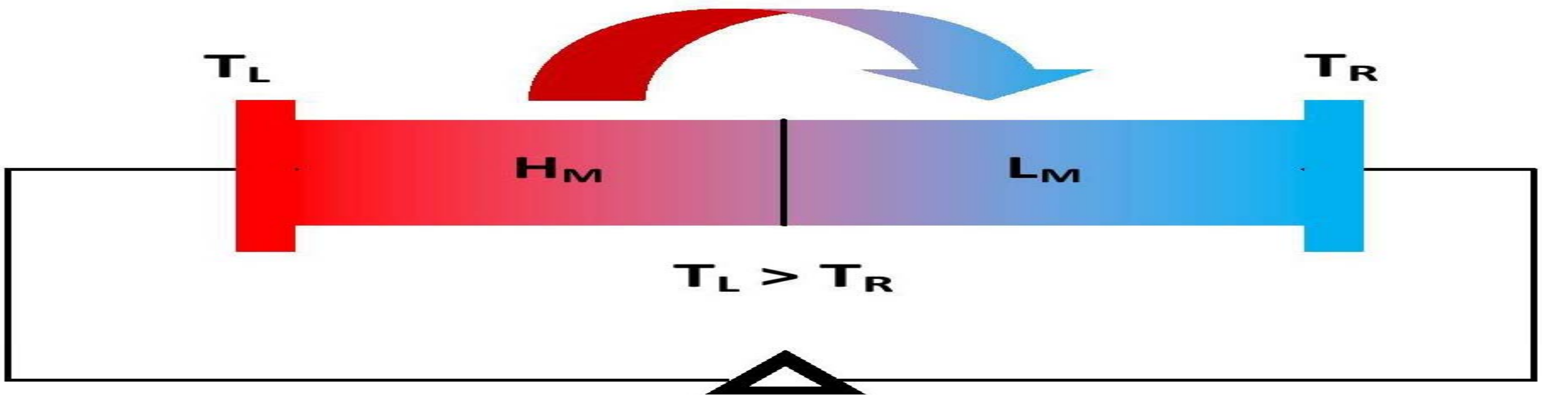
20
15
10
5
κ
0
20
40
60
80
100
N_L

Mass Effect

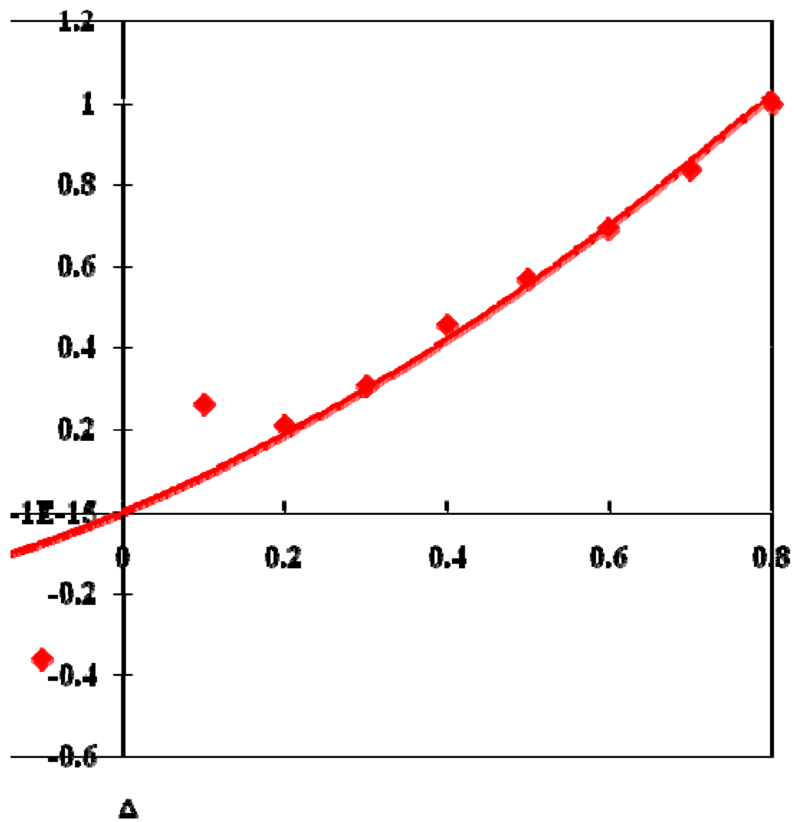


MR=0.1
MR=0.5
MR=1
MR=1.5
MR=2
MR=2.5
1.1
1.08
1.06
1.04
1.02
1
0.98
0.96
0.94
0.92
0.9
T
0
20
40
60
80
100
N

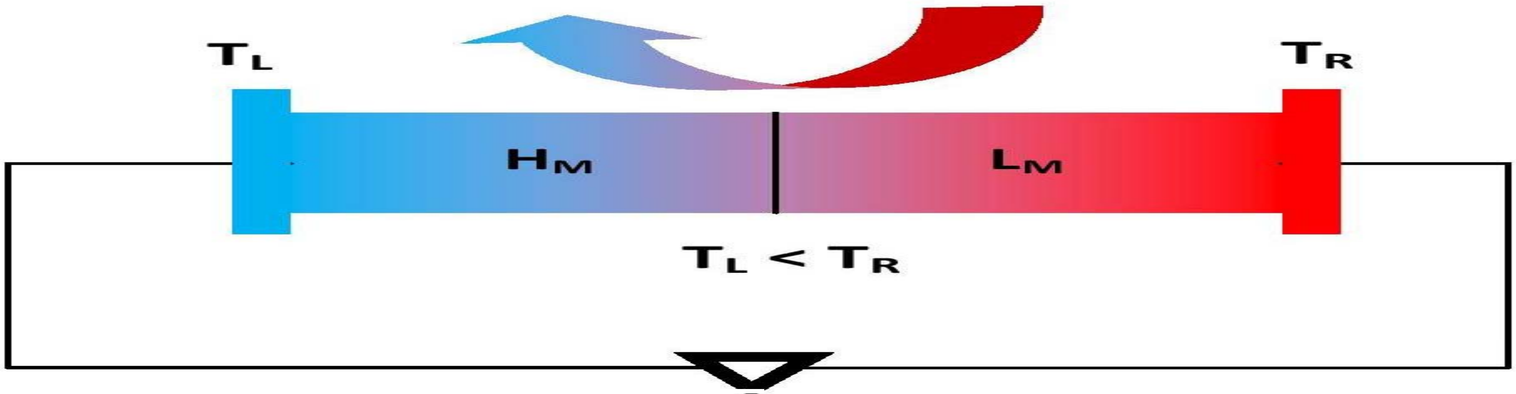

R
5.00
4.00
3.00
2.00
1.00
0.00
0
0.5
1
1.5
2
2.5
M_R/M_L
J
0.025
0.02
0.015
0.01
0
0.5
1
1.5
2
2.5
M_R/M_L
κ
20
18
16
14
12
10
0
0.5
1
1.5
2
2.5
M_R/M_L

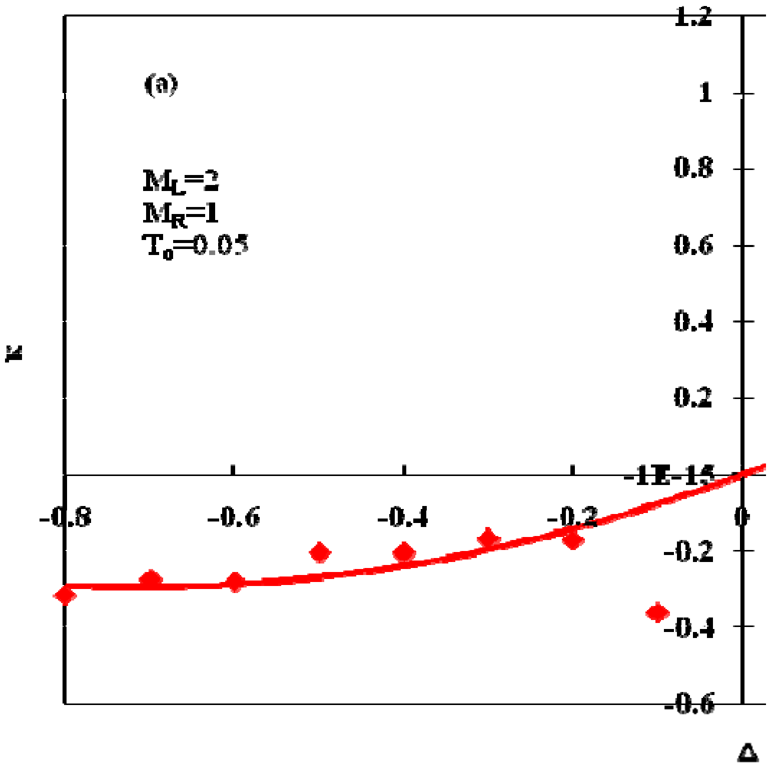


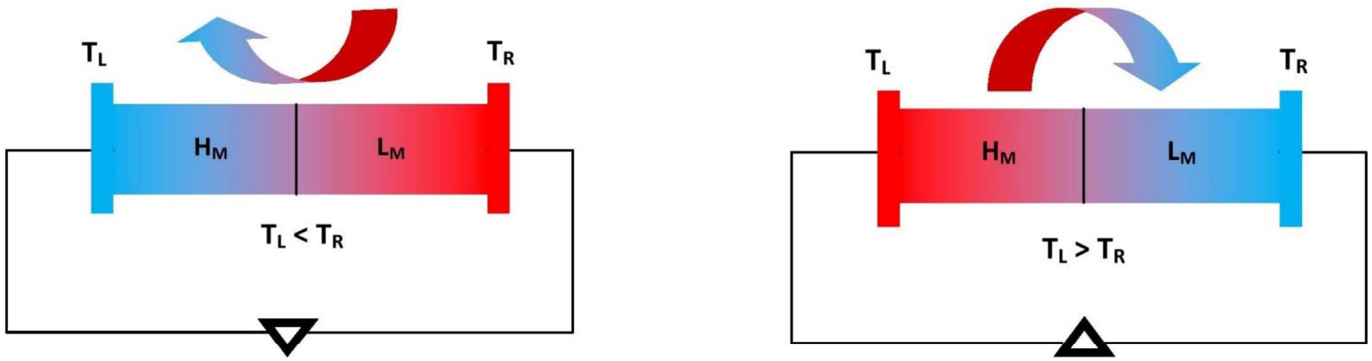
TL
TR
HM
LM
TL > TR

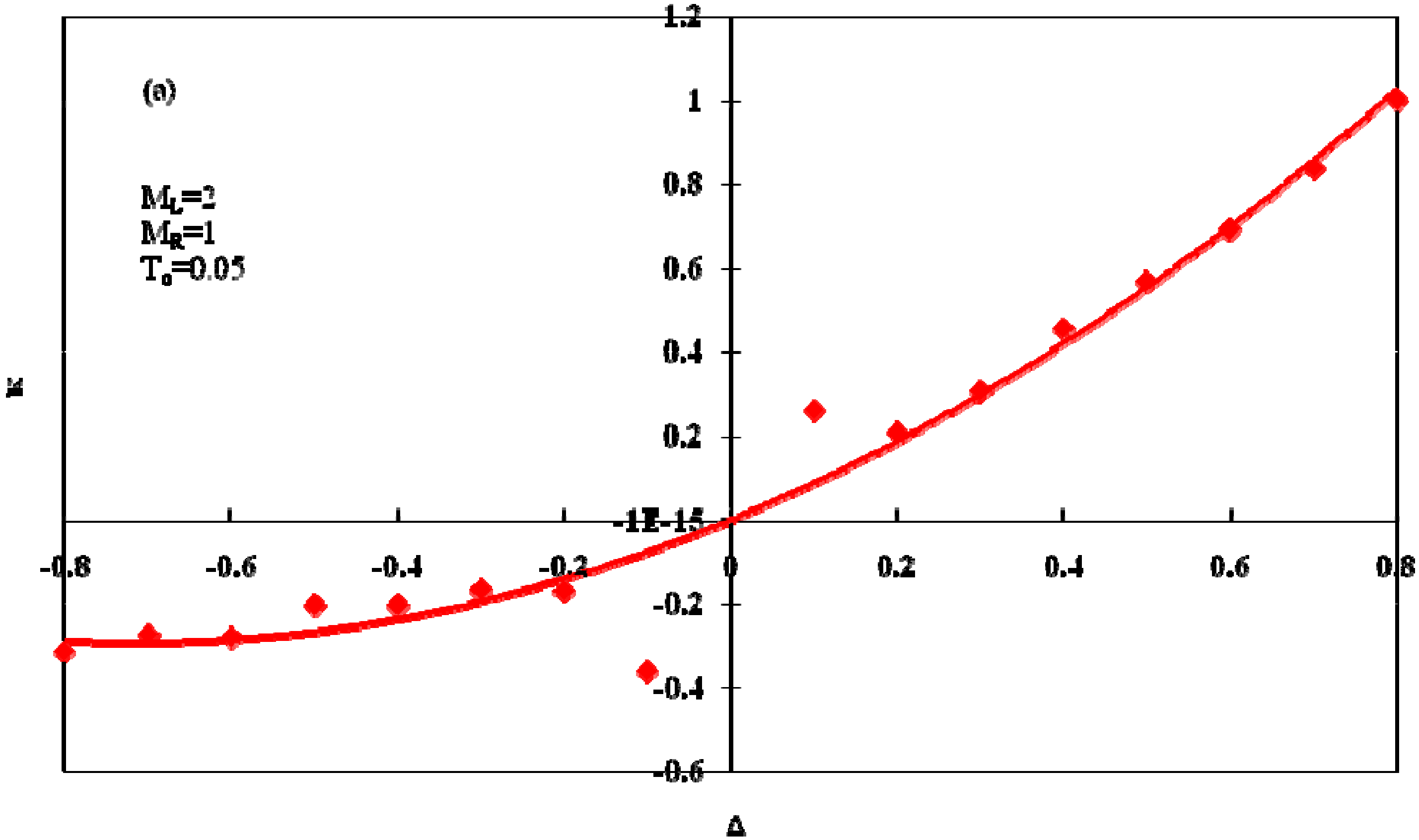


1.2
1
0.8
0.6
0.4
0.2
-1E-15
-0.2
-0.4
-0.6
0
0.2
0.4
0.6
0.8
Δ


T_L
T_R
H_M
L_M
T_L < T_R


(a)
M_L=2
M_R=1
T_0=0.05
μ
Δ
1.2
1
0.8
0.6
0.4
0.2
-1E-15
-0.2
-0.4
-0.6
-0.8
-0.6
-0.4
-0.2
0

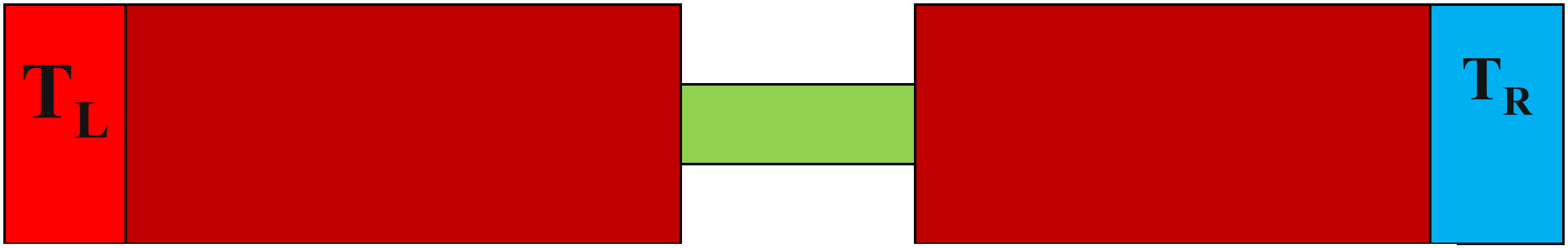

T_L
T_R
H_M
L_M
T_L < T_R
T_L
T_R
H_M
L_M
T_L > T_R

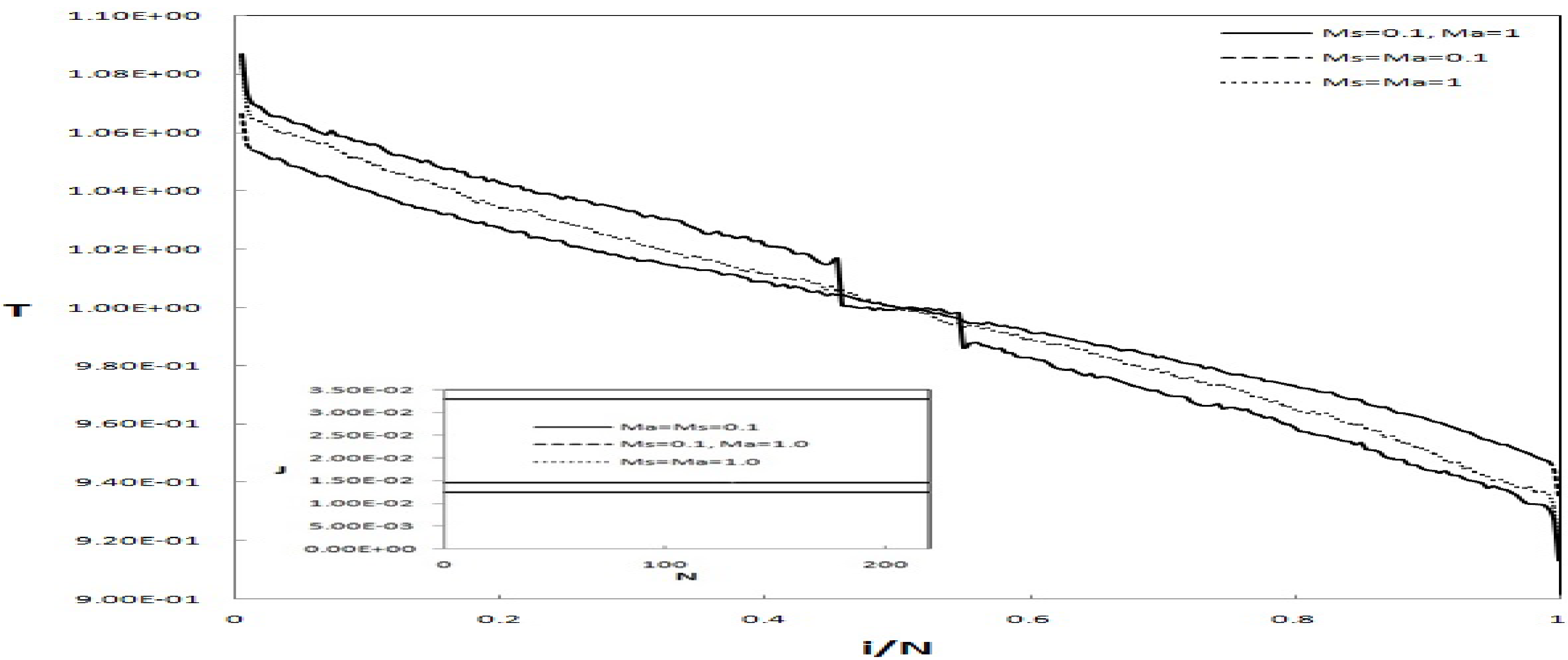

(a)
M_L=2
M_R=1
T_0=0.05
1.2
1
0.8
0.6
0.4
0.2
-1E-15
-0.2
-0.4
-0.6
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
Δ

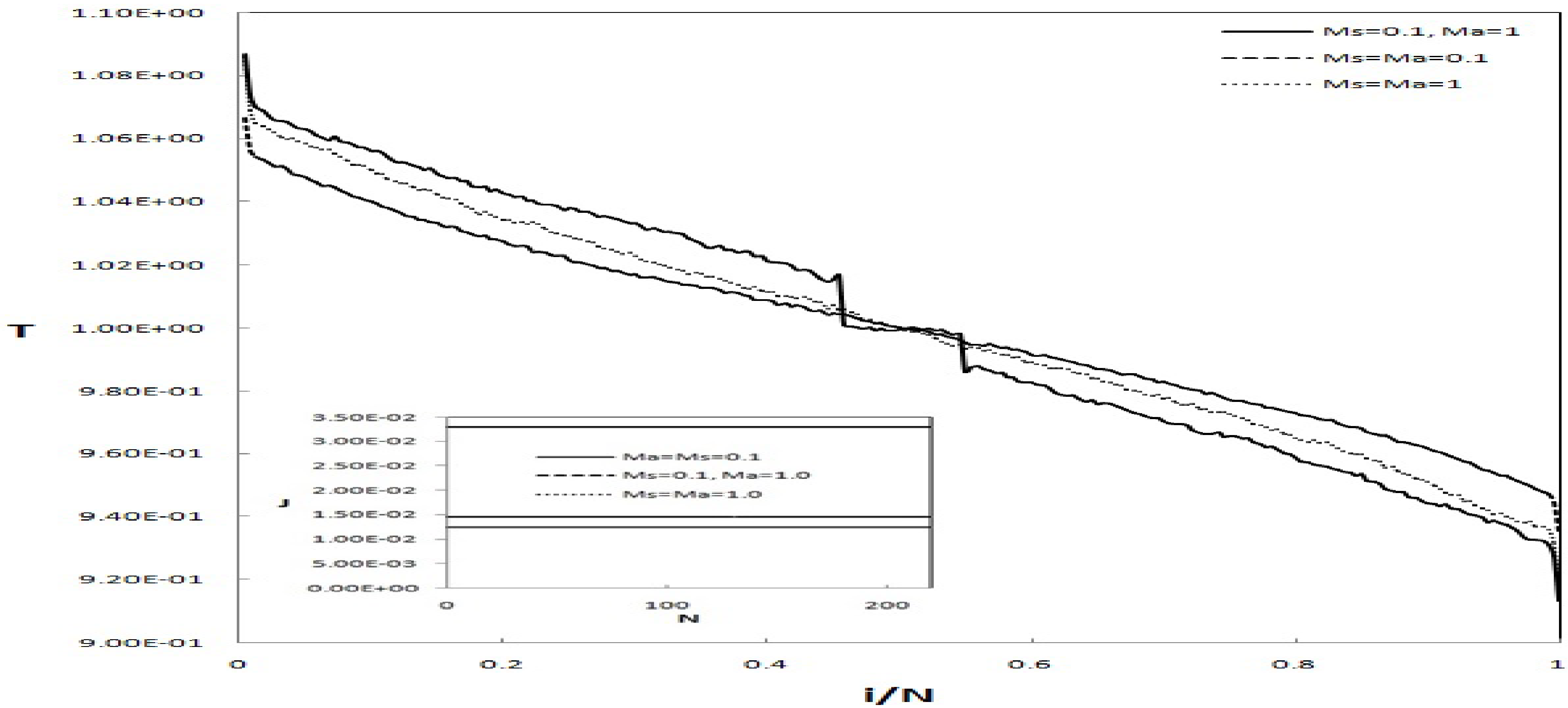
Rectification rate of Thermal Conductivity

$M_L : M_R$	T_o	κ_+	κ_-	Rectification rate κ_- / κ_+ (in %)
1:0.5	0.05	48.657	45.898	94.3
	0.1	39.637	37.125	93.6
2:1	0.05	40.059	35.391	113.1
	0.1	32.345	27.982	115.5

1D Sandwitch Structure
Tarika K. Patel & P. N. Gajjar, 2015

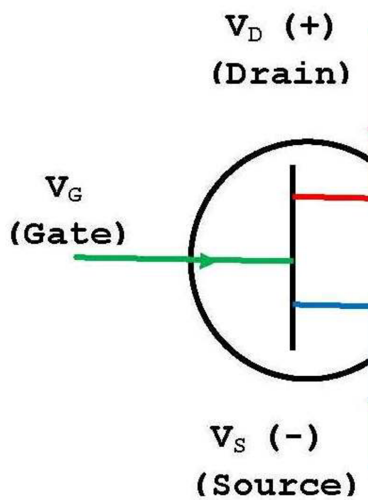


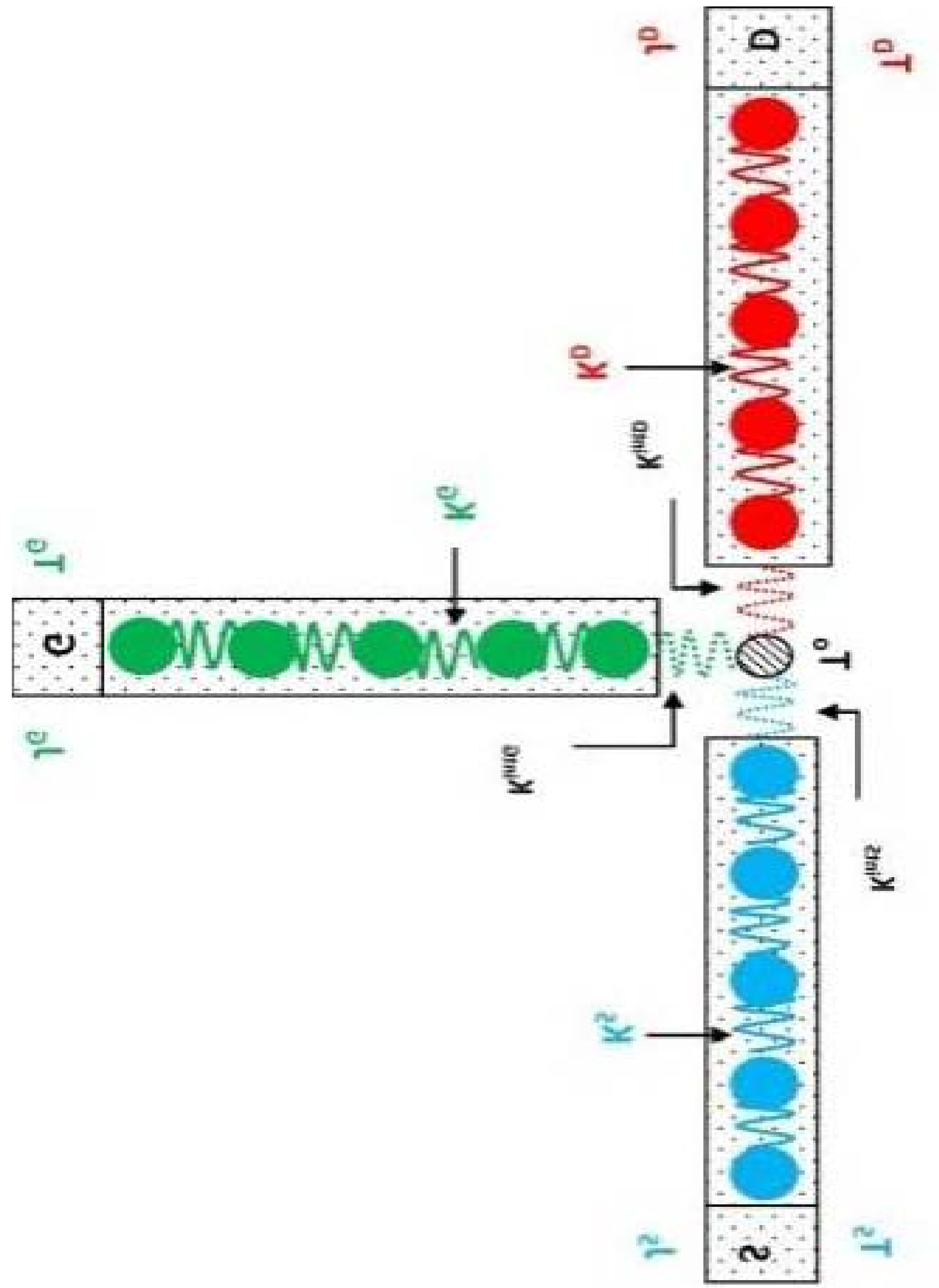




M_s	M_a	Temperature gradient		Interface Thermal Resistance		Thermal conductivity
		First interface	Second interface	First interface	Second interface	
1.0	1.0					23.319
0.1	0.1					64.764
0.1	1.0	1.601E-2	1.210E-2	1.31605	0.99439	18.701

Thermal Transistor

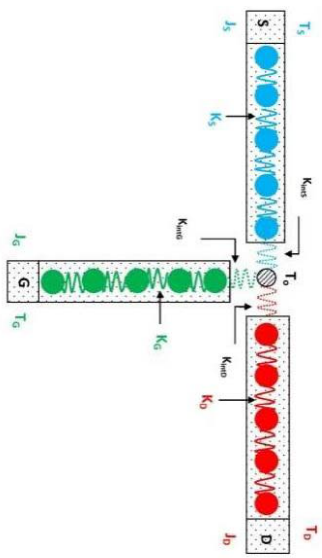


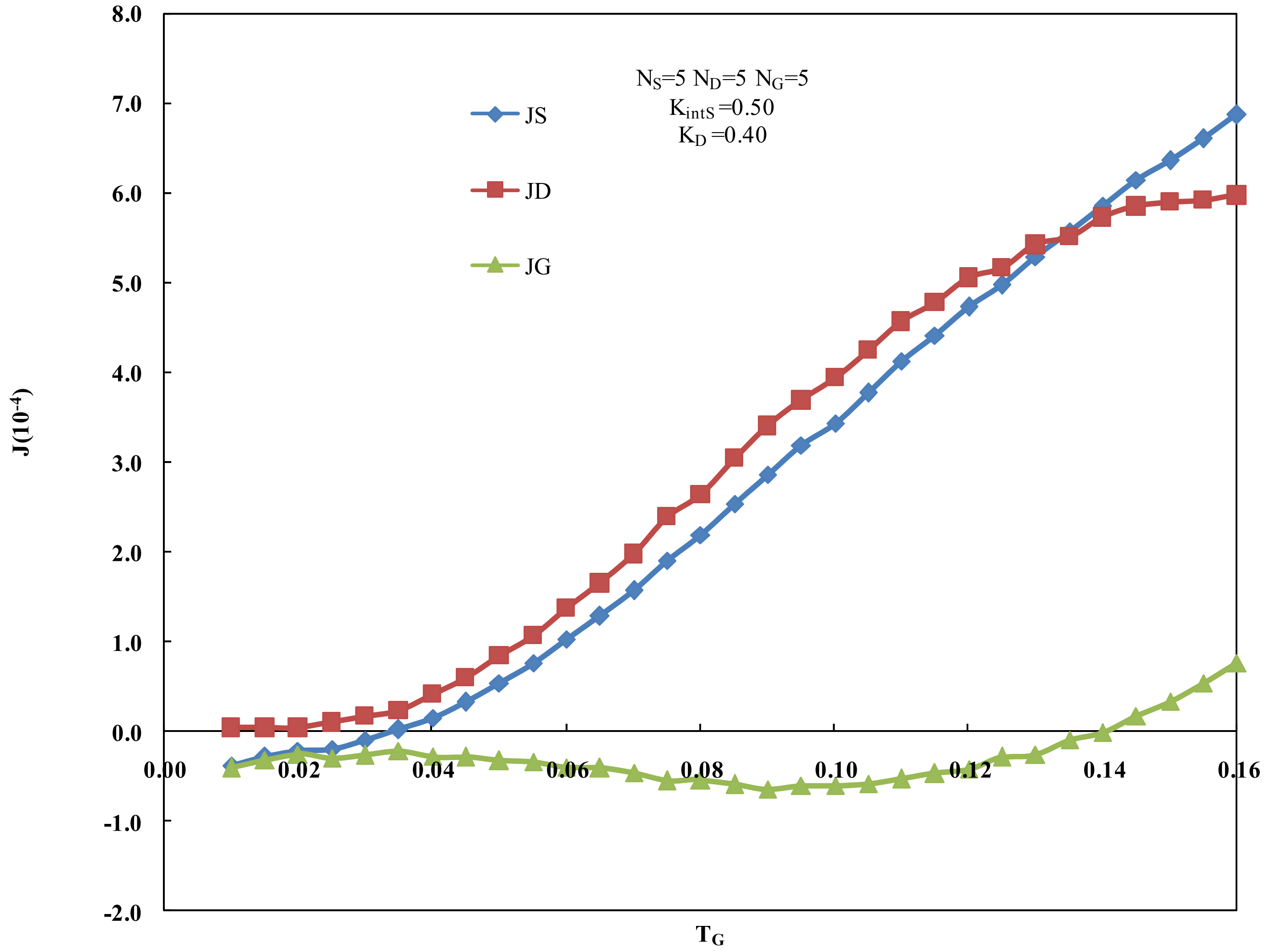


P. P. Patel & P. N. Gajjar, 2013

Thermal Transistor

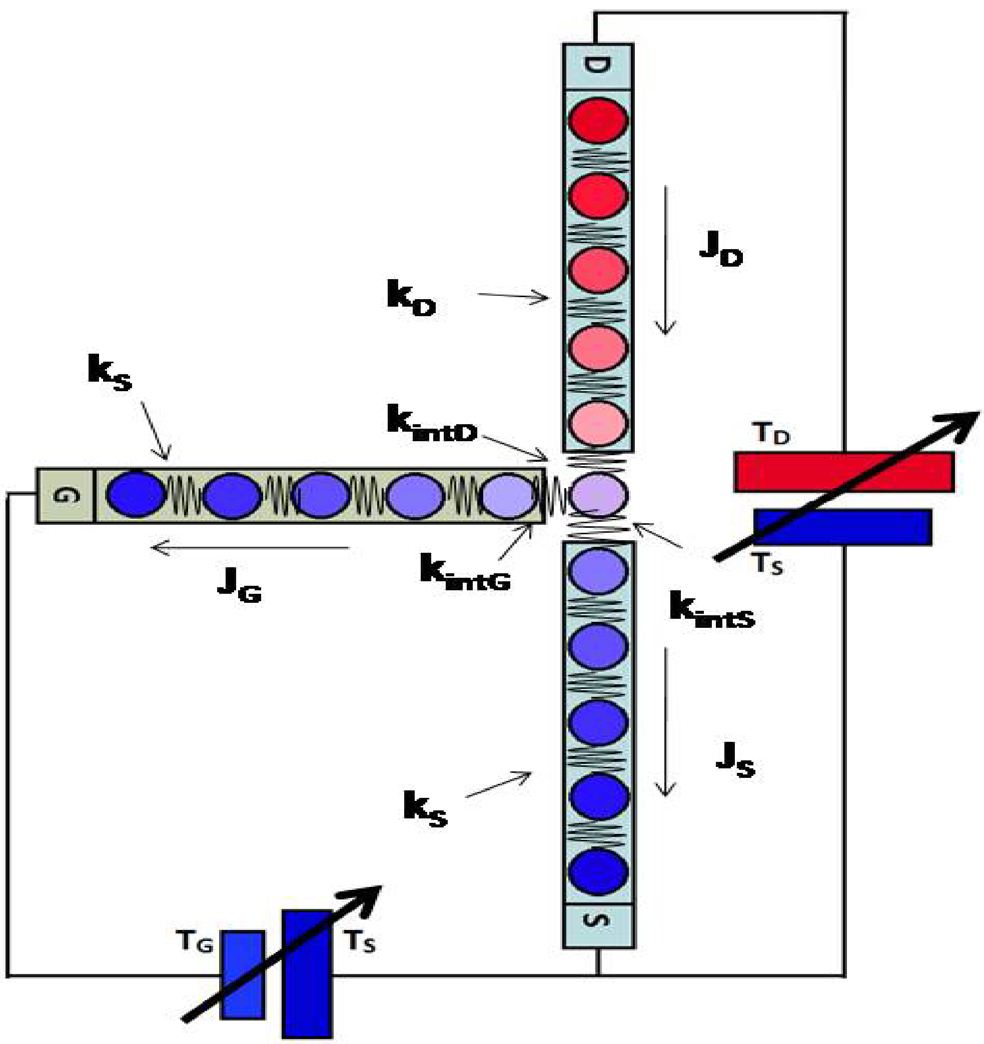
P. P. Patel & P. N. Gajjar, 2013

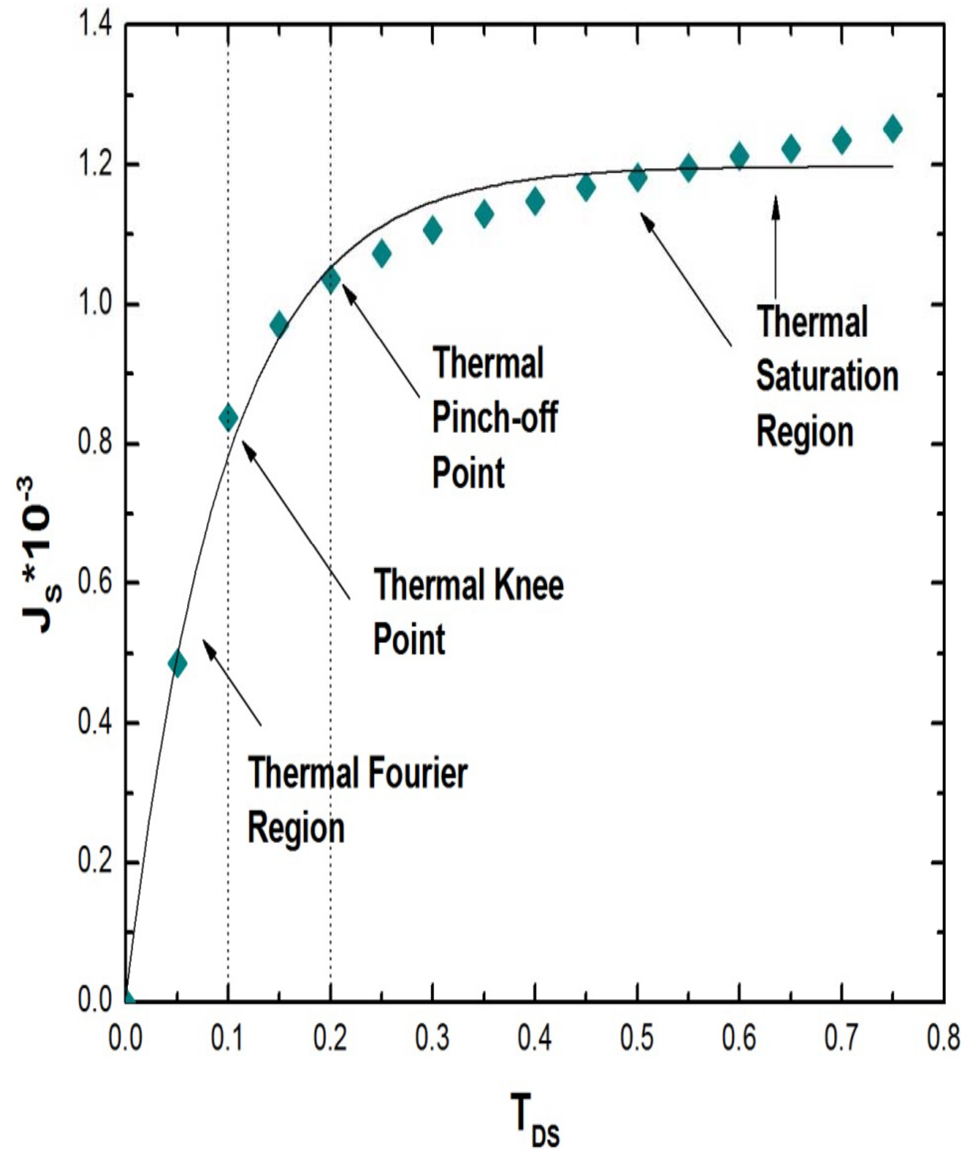




Characteristics of a Thermal Transistor

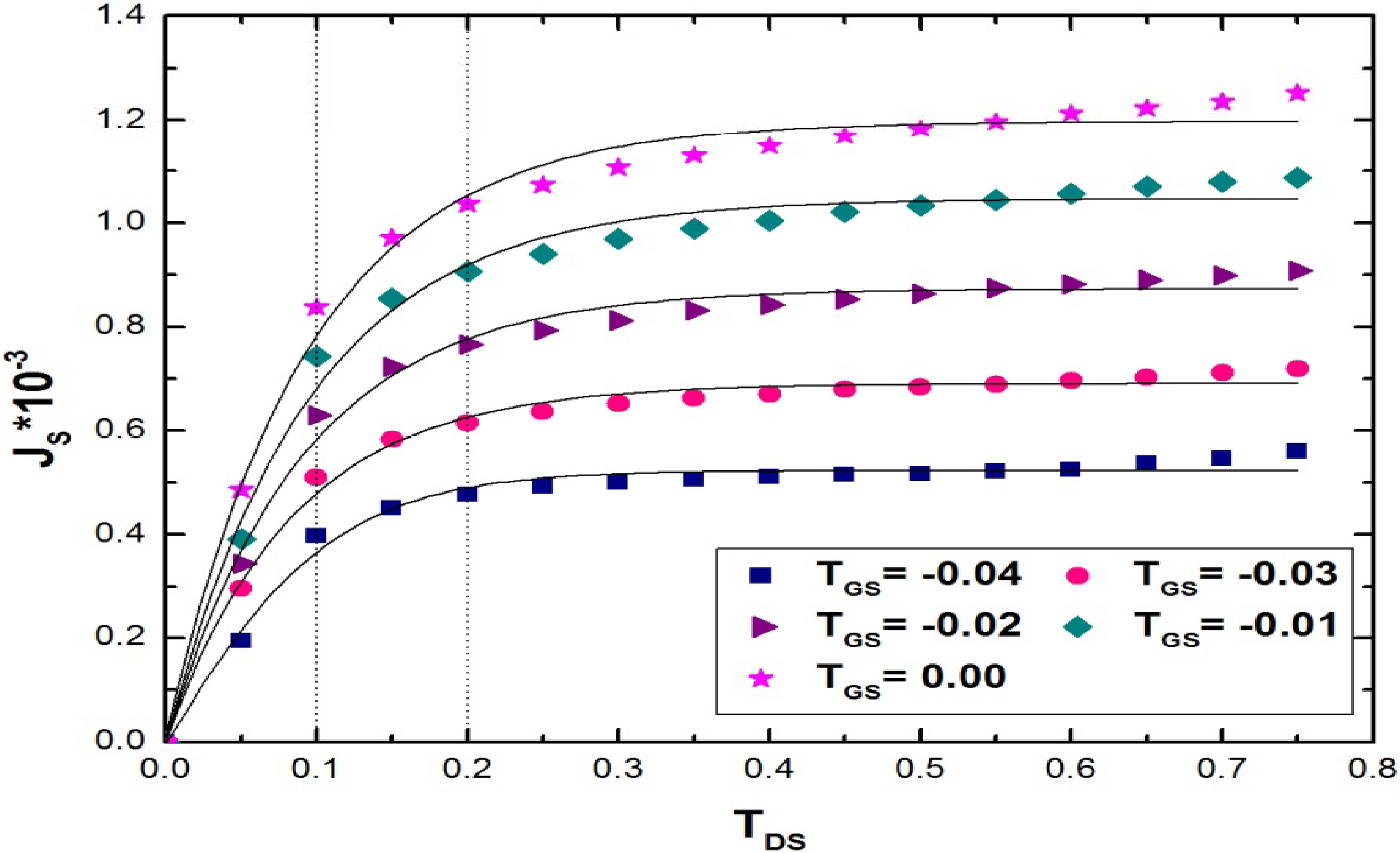
M. G. Vachhani & P. N. Gajjar (2015)





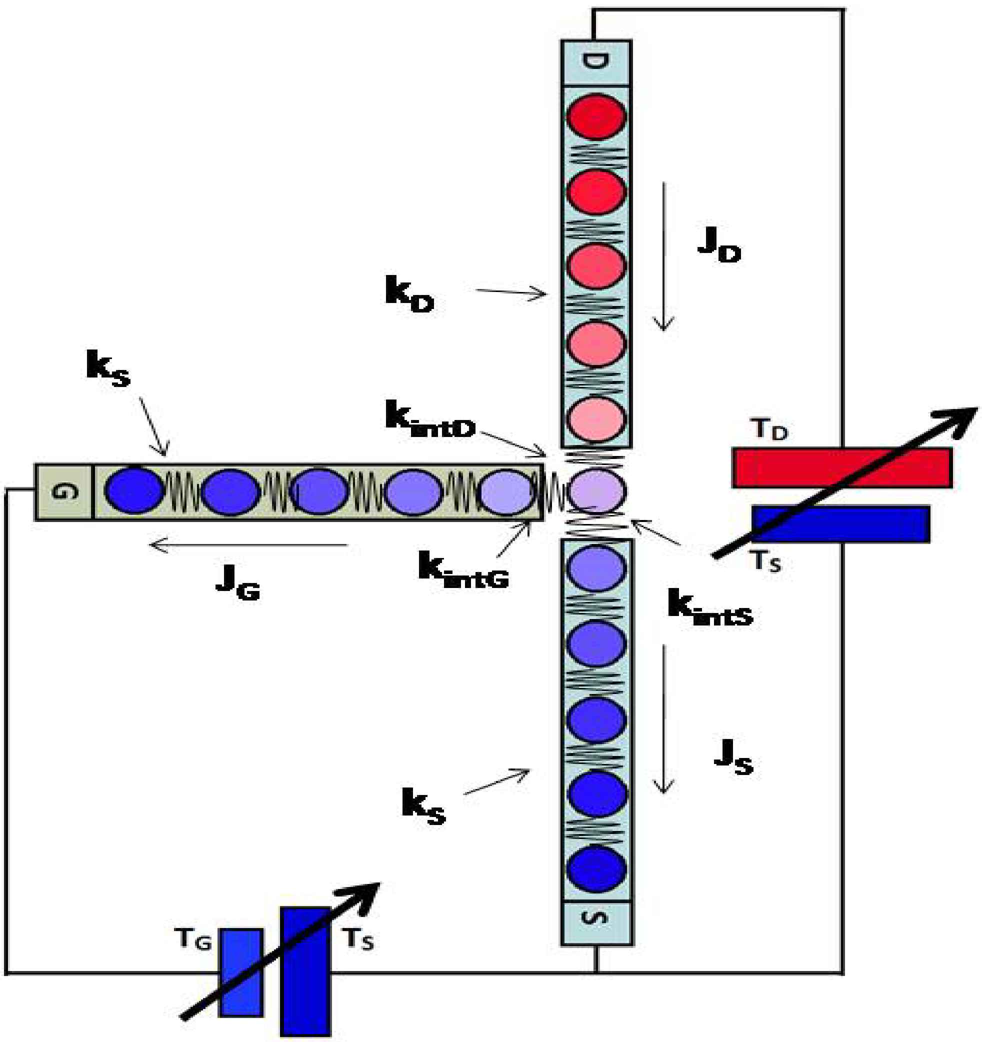
Output Characteristics of a Thermal Transistor

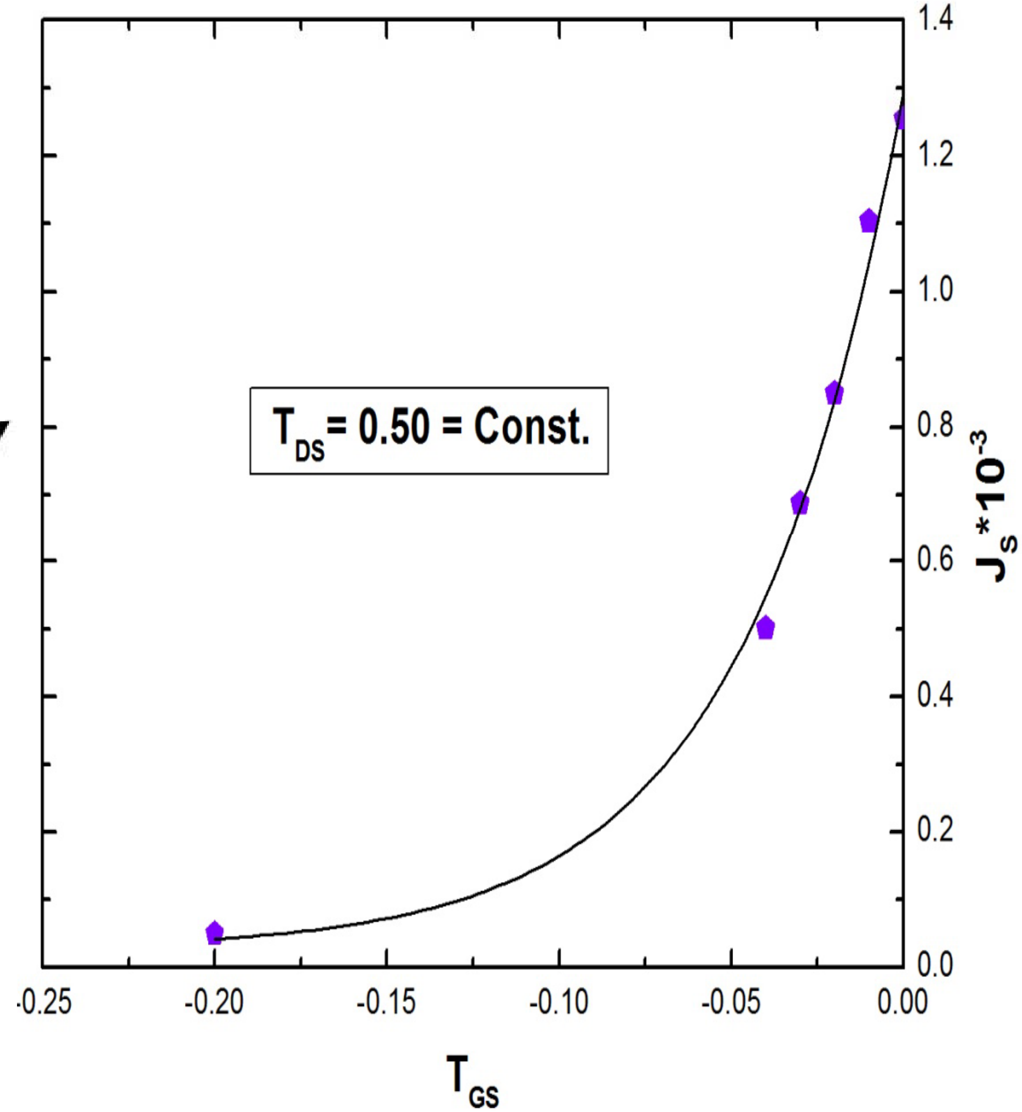
M. G. Vachhani & P. N. Gajjar (2015)



Transfer Characteristics of a Thermal Transistor

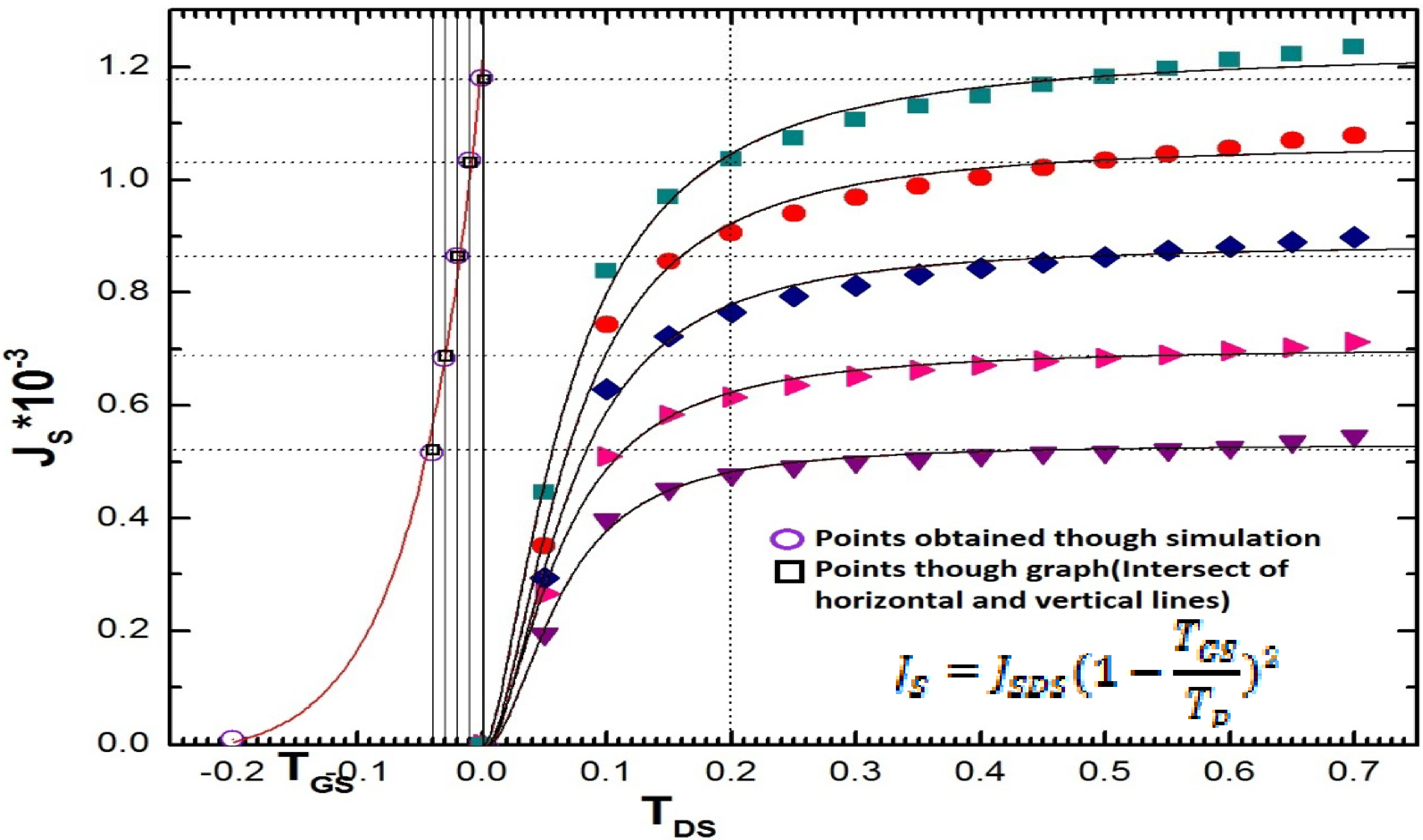
M. G. Vachhani & P. N. Gajjar (2015)





Characteristics of a Thermal Transistor

M. G. Vachhani & P. N. Gajjar (2015)



Thermal Transistor Parameters

T_{GS}=Const.	Thermal Resistance $(R_H)_S$	Thermal Resistance $(R_H)_D$	Thermal Transconductance g_m	Thermal Amplification factor μ
0.00	2.22E03	200.00	0.0164±0.0007	36.04
-0.01	3.92E03	202.02		64.29
-0.02	4.65E03	210.53		76.26
-0.03	7.41E03	250.00		121.52
-0.04	1.33E04	384.62		218.12

Why To Study Heat Transport?

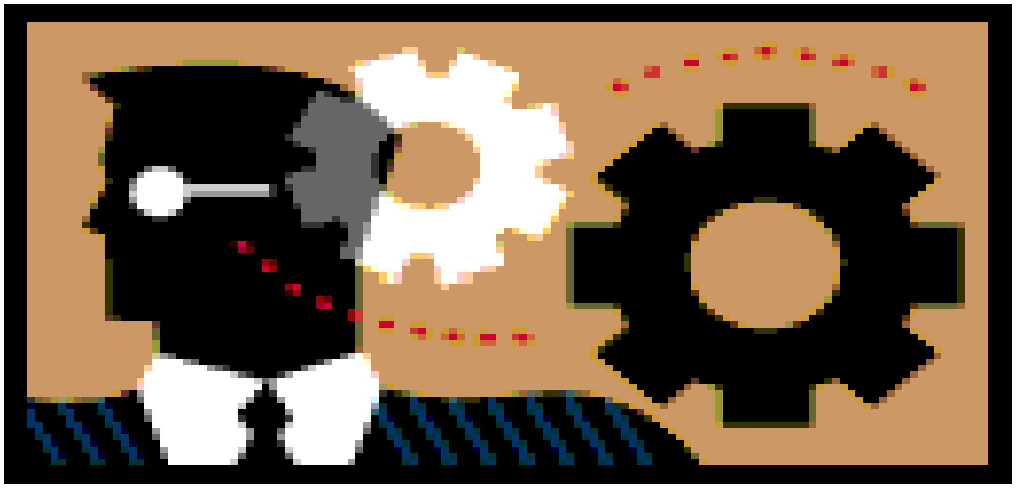
- It is to our surprise that about 90% of energy consumption of the world is either through heating or cooling.

- Looking to the amount of energy consumption in the form of heat, it is utmost essential to control / manipulate heat flow in the way we desire for the applications of heating, cooling and energy conversion.

- **The <u>first-most requirement</u> to utilize the heat is to have a material which allows us to *<u>control the flow of heat</u>* in a desire direction and/or which stores the heat for longer period of time.**

For this I have to think very differently!

- Now, I have to focus not on the photons nor on the electrons.
- But I have to follow the *PHONONS* very carefully and seriously.



THANKS

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