Peculiarities of Predicted Temperature Dependence of Nanometer Particle Mobilities

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- The model of the size-mobility relation
  Tammet, H. (1995) Size and mobility of nanometer particles, clusters and ions, *J. Aerosol Sci.* **26**, 459–475.
- Temperature variation of the mobility according to the model.
- Peculiarities of the temperature variation.
- Importance of the law of temperature variation of the mobility.

Diffusion coefficient

Mechanical mobility

$$D = kTB$$

Boltzmann constant

Temperature

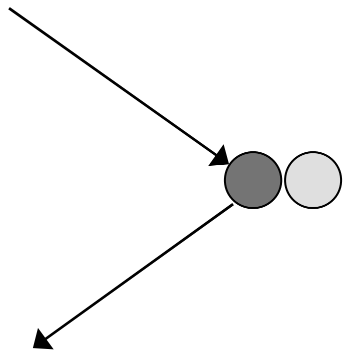
$$K = qB$$

Electrical mobility

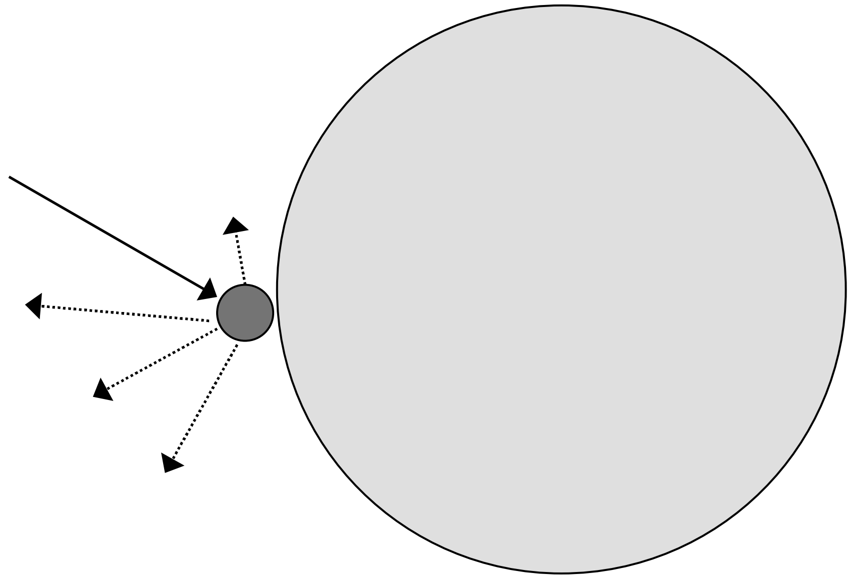
Particle charge

Well-known facts:

- A collision between a gas molecule and another molecule or small cluster is elastic-specular.



- A collision between a gas molecule and a macroscopic body (particle) is inelastic.



- **The mobility of a particle depends on the character of collisions.**

See:

Annis, B.K., Malinauskas, A.P., and Mason, E.A. (1972) Theory of drag on neutral or charged spherical aerosol particles. *J. Aerosol Sci.* **3**, 55–64.

Transition from elastic to inelastic collisions
(nanometer size range)

Formal mathematical approximations:

(1) Tammet, H. (1988) *Proc. 8th Int. Conf. Atmos. Electricity*, Uppsala, pp. 21–30.

(2) Ramamurthi, M. and Hopke, P.K. (1989) *Health Physics* **56**, 189–194.

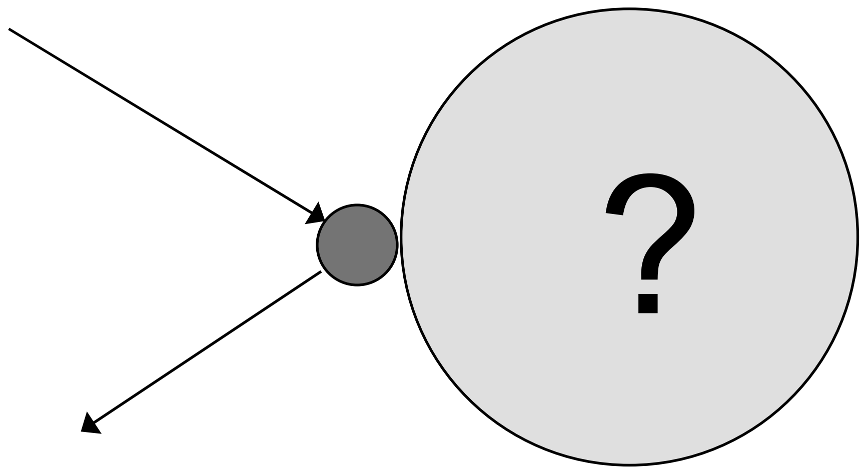
Physical hypothesis:

(3) Tammet, H. (1995) *J. Aerosol Sci.* **26**, 459–475.

Indirect experimental data:

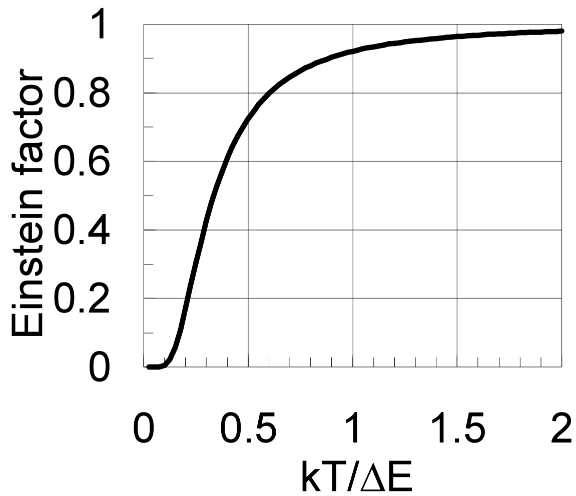
Kilpatrick, W.D. (1971) An experimental mass-mobility relation for ions in air at atmospheric pressure. *Proc. 19th Annu. Conf. Mass Spectrosc.,* pp. 320–325.

$$d_m = \sqrt[3]{\frac{6m}{\pi\rho}} \qquad r_m = \frac{d_m}{2}$$



The Einstein factor of melting of the internal degrees of freedom:

$$\left(\frac{\Delta E}{kT}\right)^2 \frac{\exp\left(\frac{\Delta E}{kT}\right)}{\left(\exp\left(\frac{\Delta E}{kT}\right)-1\right)^2}$$



ΔE – separation of the internal energy levels,
N – number of atoms in the particle,
d_m and r_m – mass diameter and mass radius.

$$d_m = \sqrt[3]{\frac{6m}{\pi\rho}} \qquad r_m = \frac{d_m}{2} \qquad \overline{\Delta E} = \frac{\text{const}_1}{N} = \frac{\text{const}_2}{r_m^3}$$

Importance:

1) *verification of the model,*
2) *reduction of the mobilities,*
3) *distinction between particles and clusters.*

....

Langevin reduction used by Kilpatrick:

$$K_{\mathrm{reduced}} = K_{\mathrm{measured}} \frac{273.15\mathrm{K}}{T} \frac{p}{101325\mathrm{Pa}}$$

$$K \approx \left(\sqrt[3]{\frac{850\mathrm{u}}{m}} - 0.3 \right) \mathrm{cm}^2 \mathrm{V}^{-1} \mathrm{s}^{-1}$$

CRC Handbook of Physics and Chemistry (1993), 74th edition.

Corrected reduction:

$$K_{\mathrm{measured}} \rightarrow d_m \rightarrow K_{\mathrm{reduced}}$$

$$K \approx \left(\sqrt[3]{\frac{1210\mathrm{u}}{m}} - 0.21 \right) \mathrm{cm}^2 \mathrm{V}^{-1} \mathrm{s}^{-1}$$

Distinction between

MACROSCOPIC PARTICLES

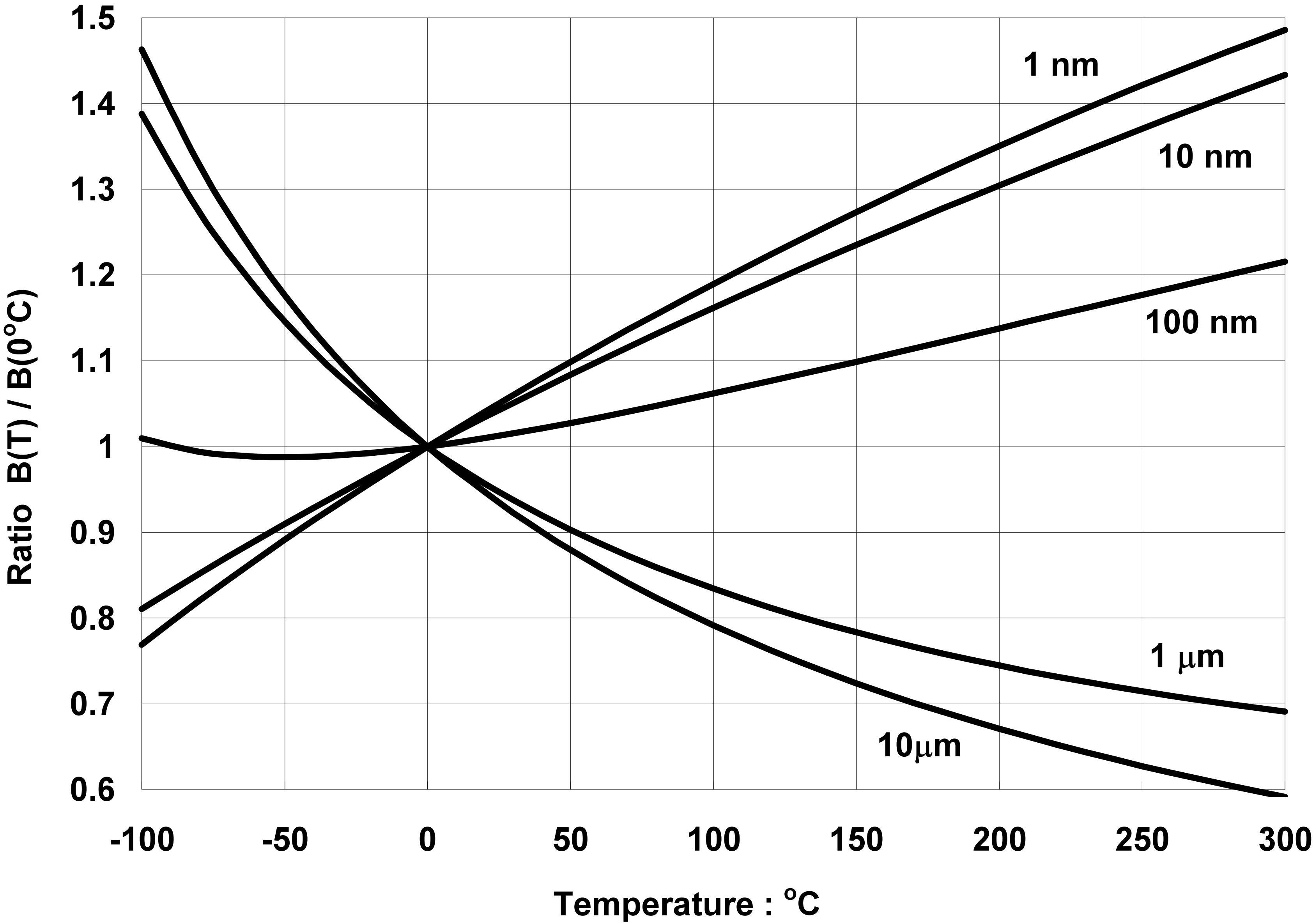
and

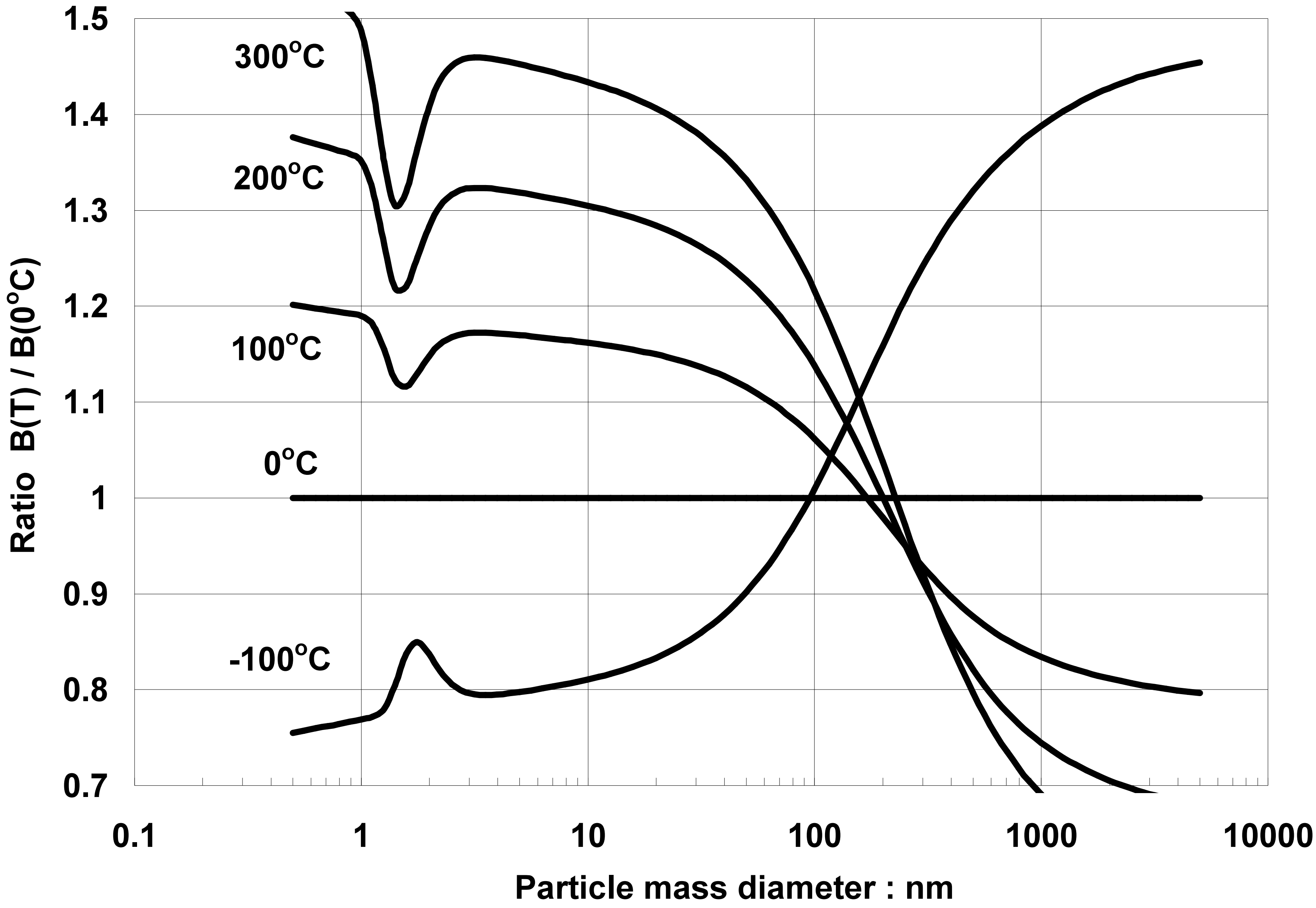
MOLECULAR CLUSTERS

According to the long term measurements of atmospheric ions the mobility of 0.5 $cm^2V^{-1}s^{-1}$ appears as critical in statistical behavior of air ion fraction concentrations.

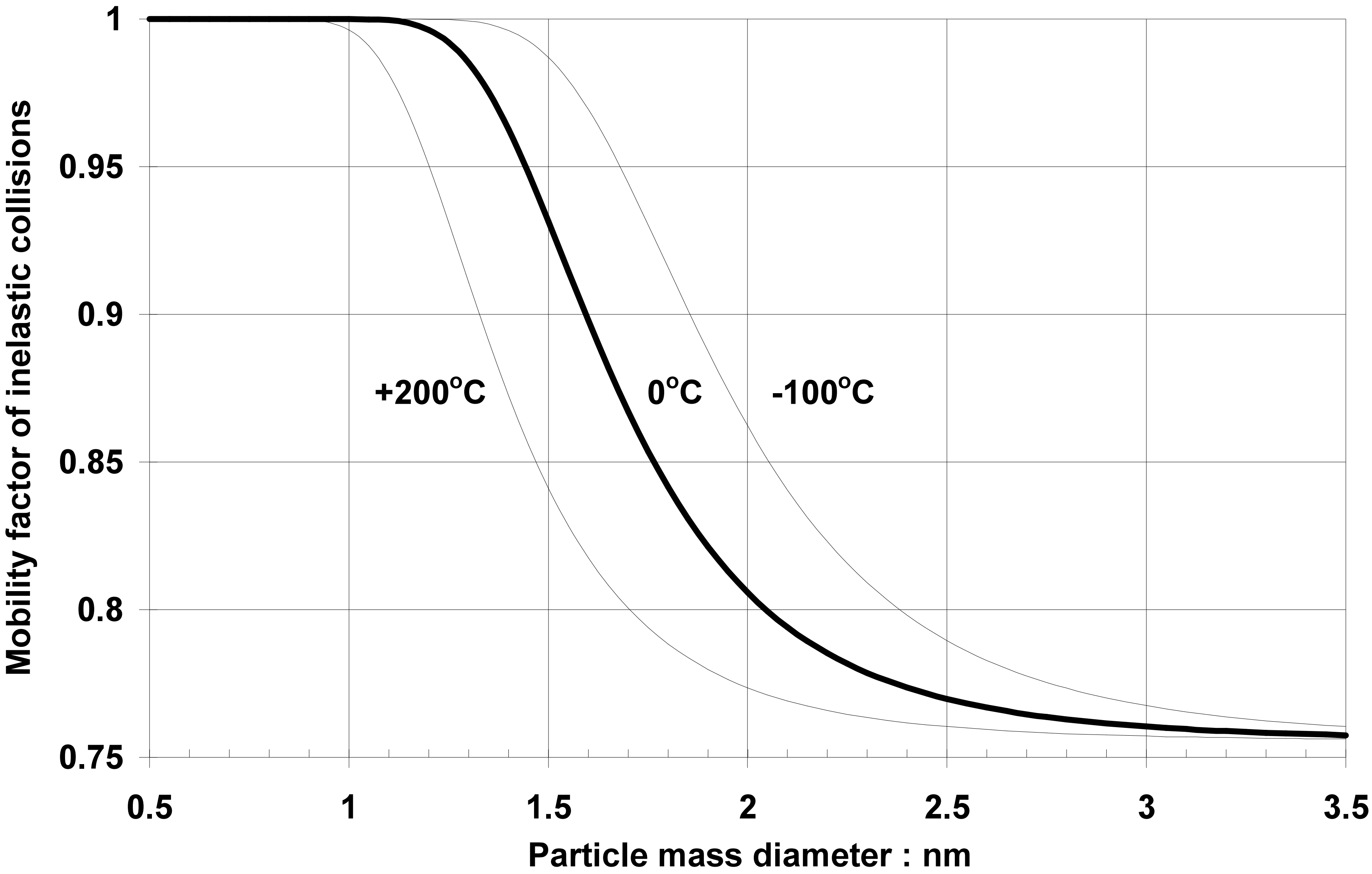
The mass diameter of critical air ions 1.6 nm is just the same as the critical diameter of the transition from elastic to inelastic collisions.

Therefore, the term *macroscopic particles* could be preferred when speaking about particles of diameter greater than 1.6 nm and the term *molecular clusters* when considering the particles of diameter less than 1.6 nm.

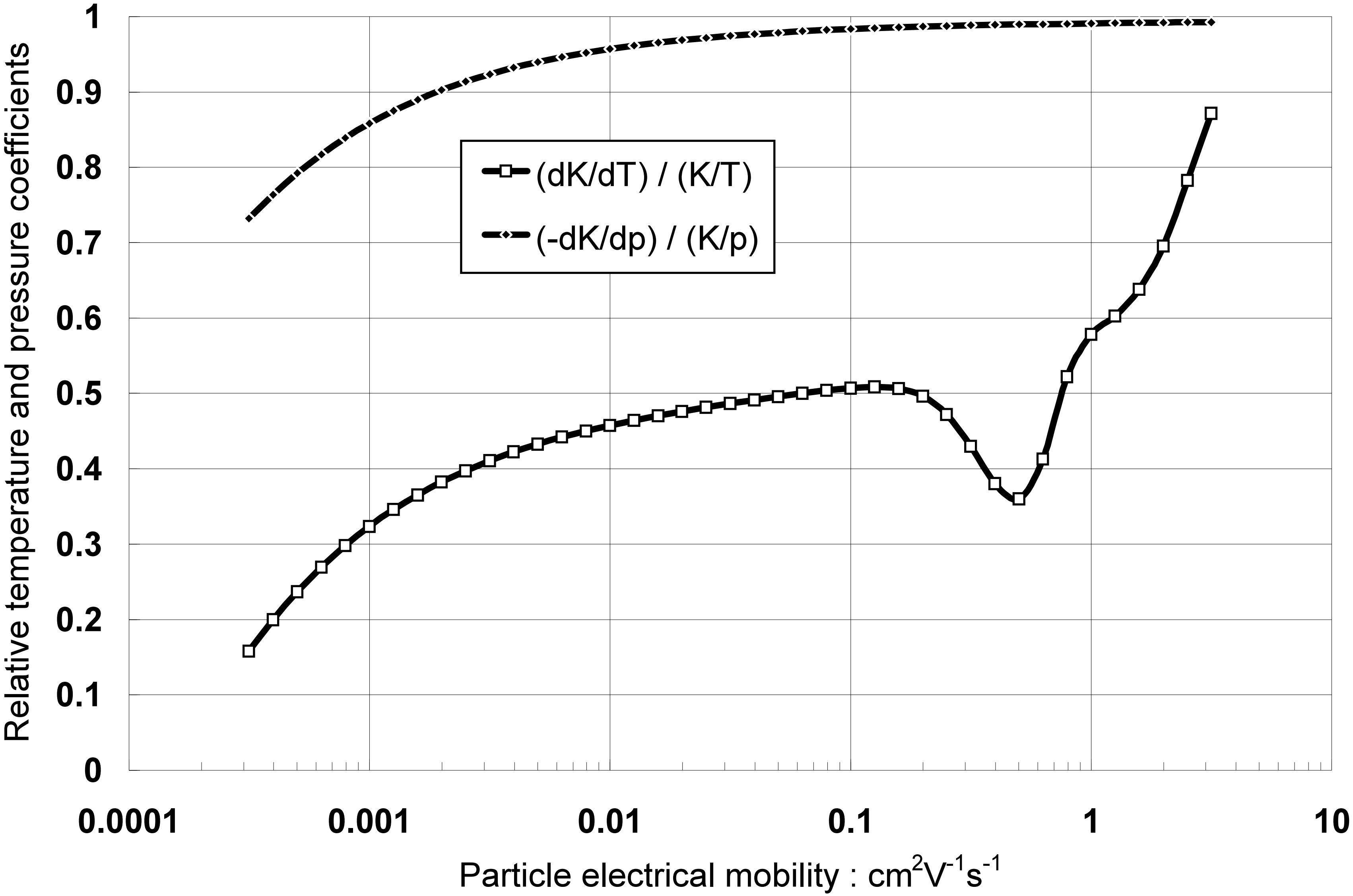

1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
Ratio B(T) / B(0°C)
-100
-50
0
50
100
150
200
250
300
Temperature : °C
1 nm
10 nm
100 nm
1 μm
10μm



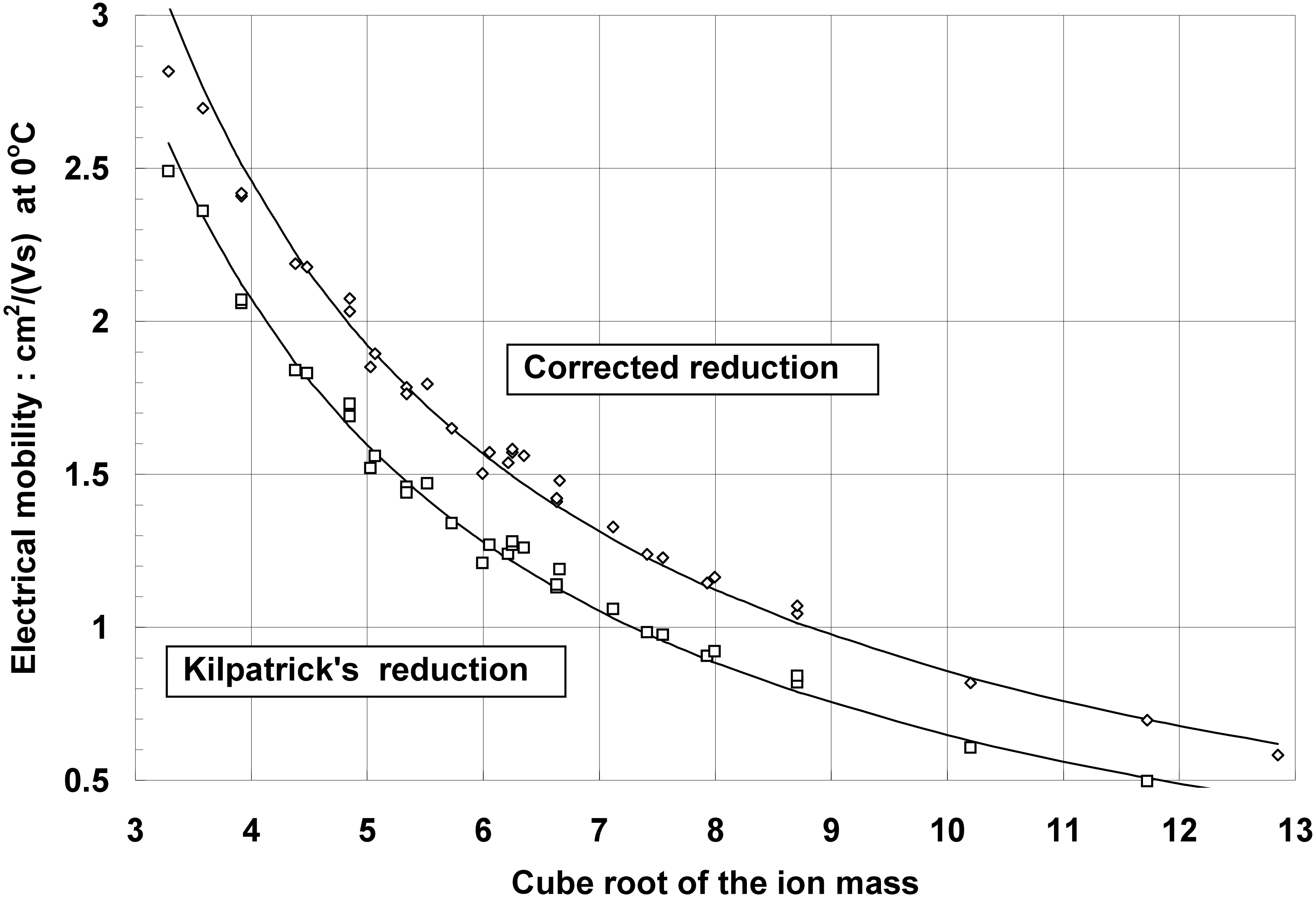
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
Ratio B(T) / B(0°C)
300°C
200°C
100°C
0°C
-100°C
0.1
1
10
100
1000
10000
Particle mass diameter : nm



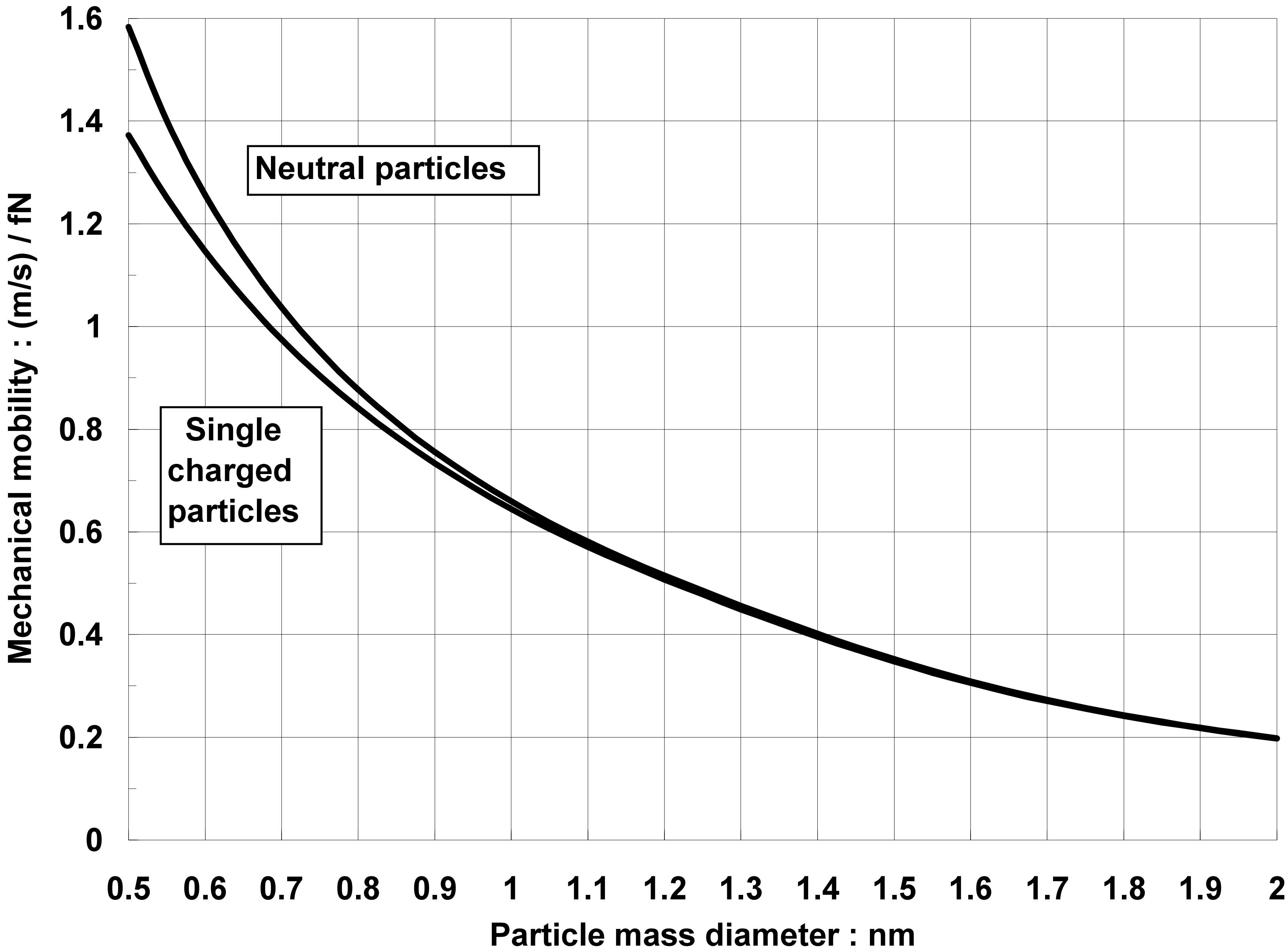
1
0.95
0.9
0.85
0.8
0.75
0.5
1
1.5
2
2.5
3
3.5
Mobility factor of inelastic collisions
Particle mass diameter : nm
+200°C
0°C
-100°C



Relative temperature and pressure coefficients
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.0001
0.001
0.01
0.1
1
10
Particle electrical mobility : cm²V⁻¹s⁻¹
(dK/dT) / (K/T)
(-dK/dp) / (K/p)



Electrical mobility : cm²/(Vs) at 0°C
3
2.5
2
1.5
1
0.5
3
4
5
6
7
8
9
10
11
12
13
Cube root of the ion mass
Corrected reduction
Kilpatrick's reduction



Neutral particles
Single charged particles
Mechanical mobility : (m/s) / fN
Particle mass diameter : nm
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2