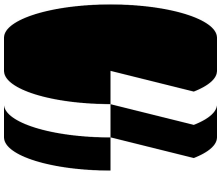
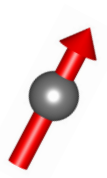
Thermal expansion

dilatometry



NTE materials

Eduard Grüneisen



by Alexander Tsirlin, Leipzig University

Lecture 15: November 30, 2023

Debye-Waller factor

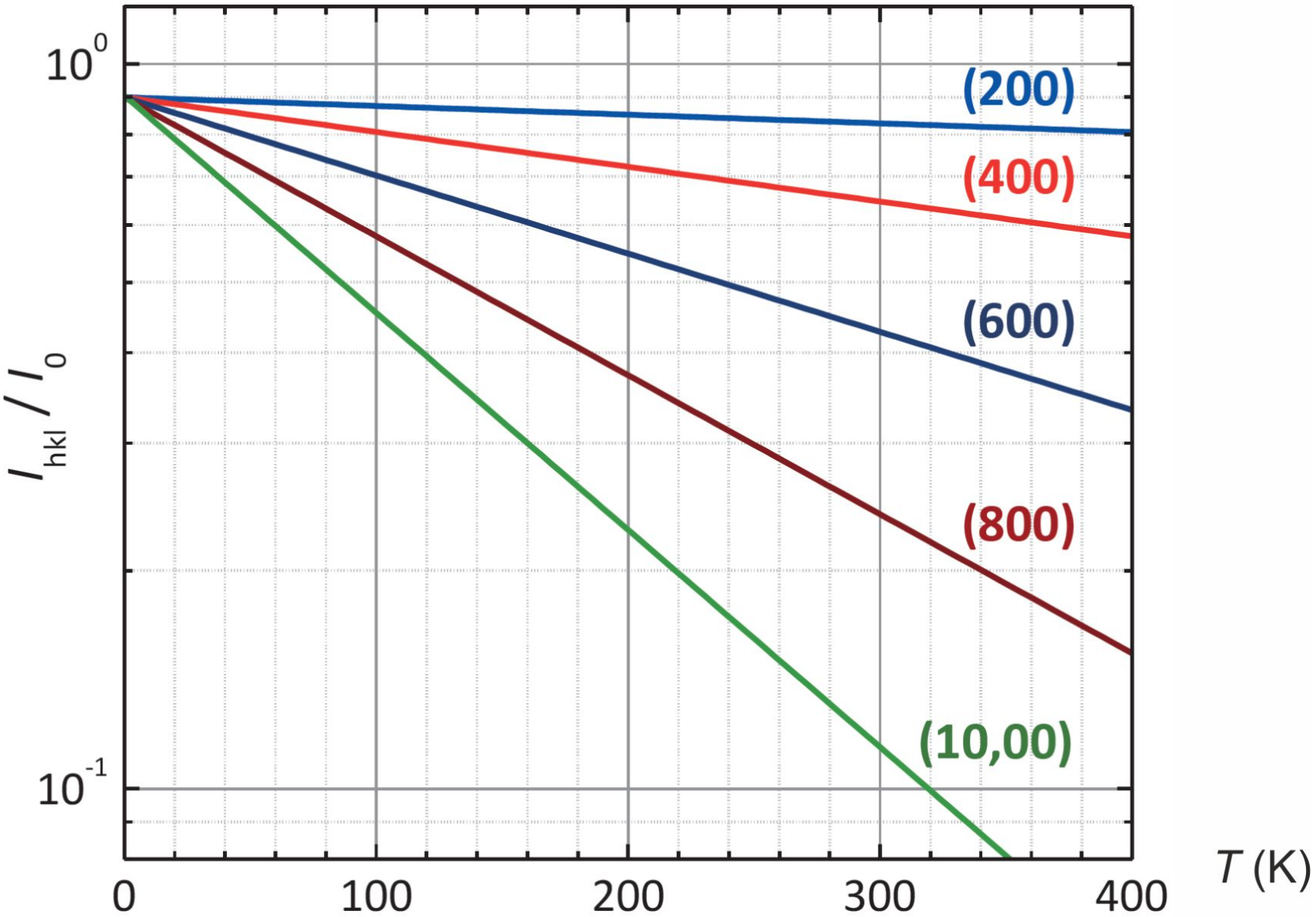


Image credit: Gross and Marx, Festkörperphysik

Debye-Waller factor

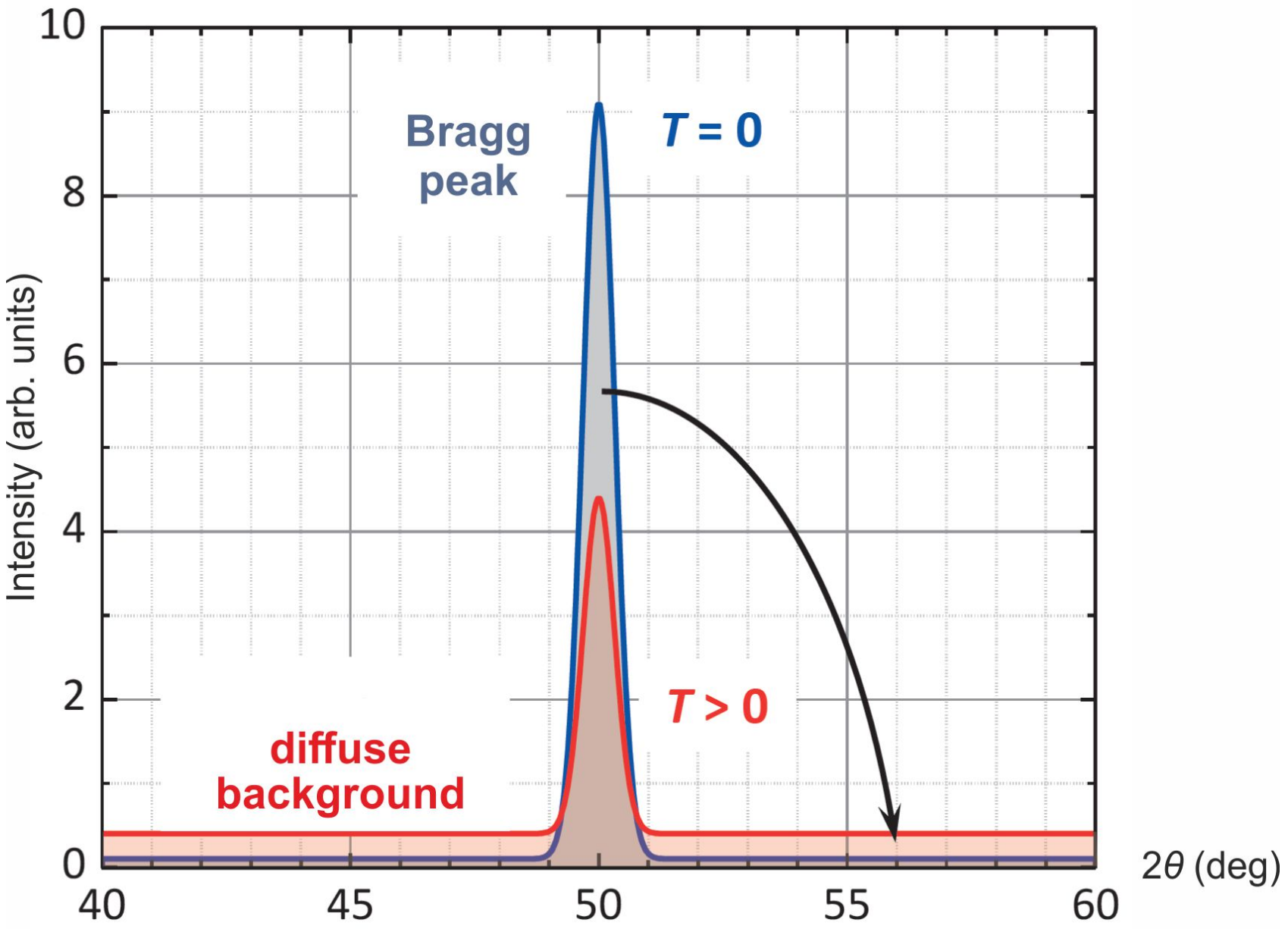
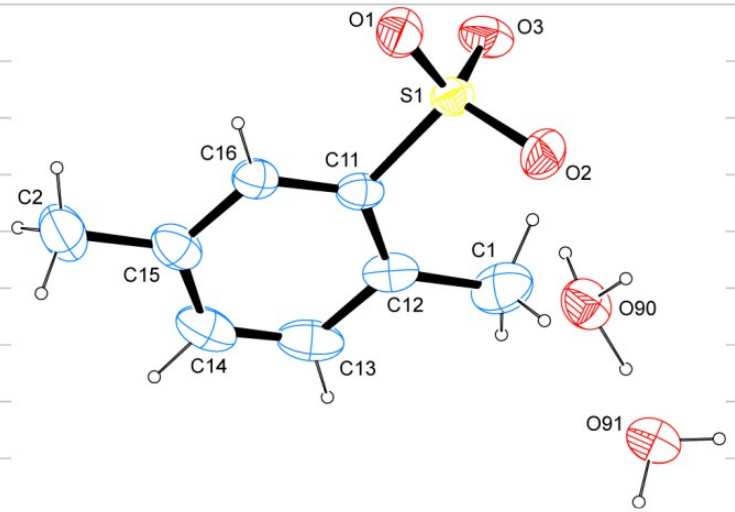


Image credit: Gross and Marx, Festkörperphysik

Atomic displacement parameter

Atom	x	y	z	U_{iso}*/U_{eq}
S1	0.25094 (6)	0.71542 (5)	0.81103 (3)	0.02902 (12)
O1	0.0450 (2)	0.7896 (2)	0.82083 (13)	0.0409 (4)
O2	0.2780 (3)	0.58300 (19)	0.90288 (14)	0.0410 (3)
O3	0.4231 (3)	0.82997 (19)	0.82379 (15)	0.0411 (4)
C1	0.6169 (4)	0.4929 (3)	0.7124 (3)	0.0509 (6)
H1A	0.657557	0.588421	0.761828	0.076*
H1B	0.736917			0.076*
H1C	0.572203			0.076*
C2	−0.0600 (4)			0.0510 (6)
H2A	0.001984			0.076*
H2B	−0.156354			0.076*
H2C	−0.137050			0.076*
C11	0.2663 (3)			0.0292 (3)
C12	0.4395 (3)			0.0365 (4)
C13	0.4386 (4)			0.0469 (5)



Every reported crystal structure should have a *U*-parameter (typically one for each atomic position)

Z. Krist. NCS 236, 511 (2021)

Expansion joints: bridges

Image credit: Ingolfson and GT1976 (CC-BY-SA)

Expansion joints: pipes

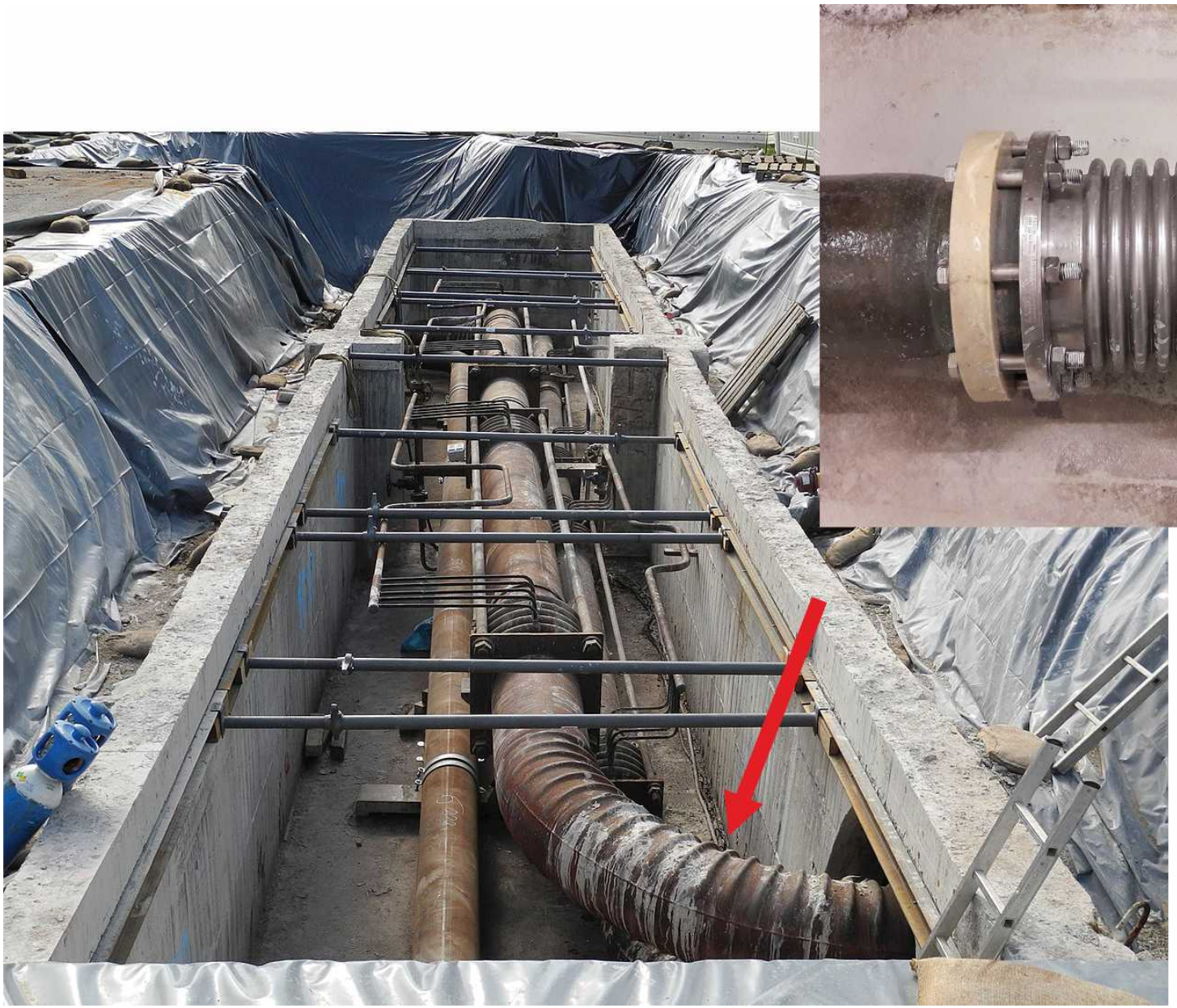


Image credit (CC-BY-SA)
RomanM82 and SchiDD

Breather switch (rails)

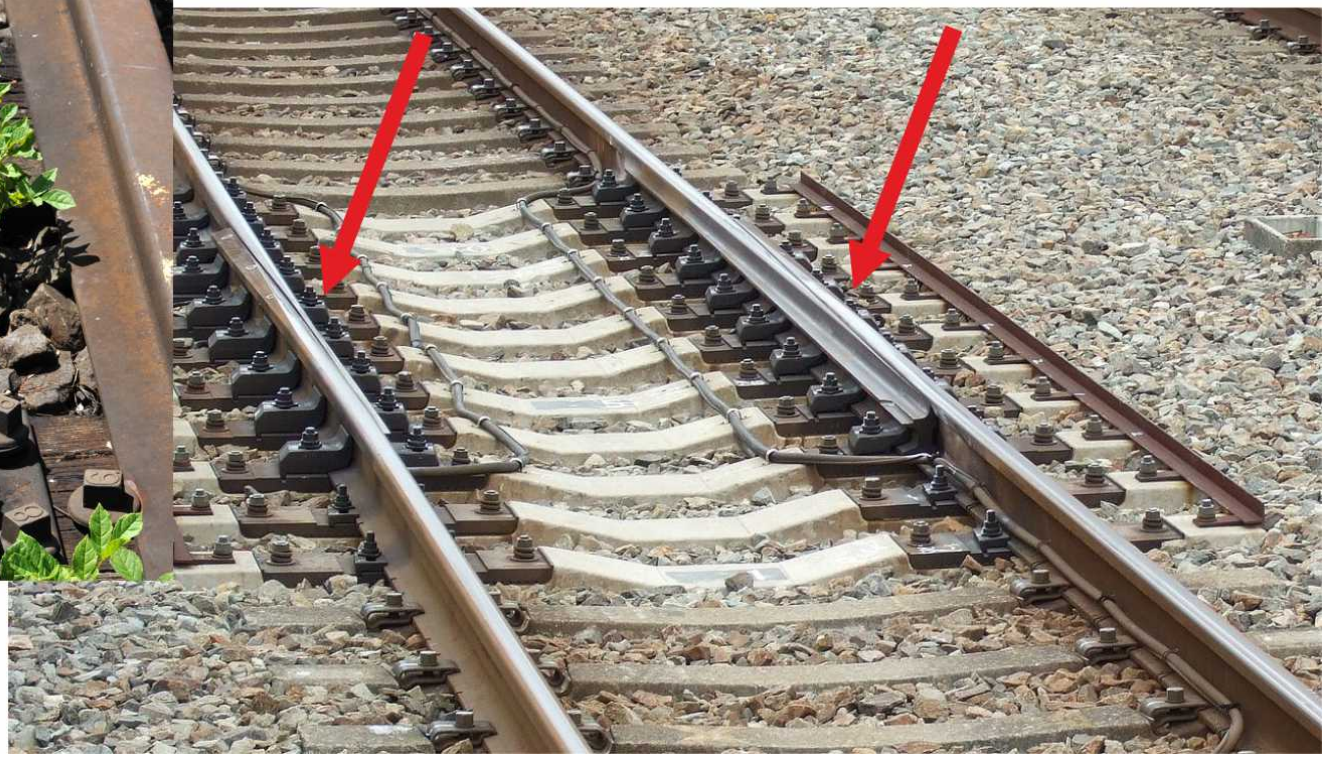


Image credit: Chriusha and Haragayato (CC-BY-SA)

Adverse effects of thermal expansion

Image credits:
ABproTWE (CC-BY-SA)

Adverse effects of thermal expansion

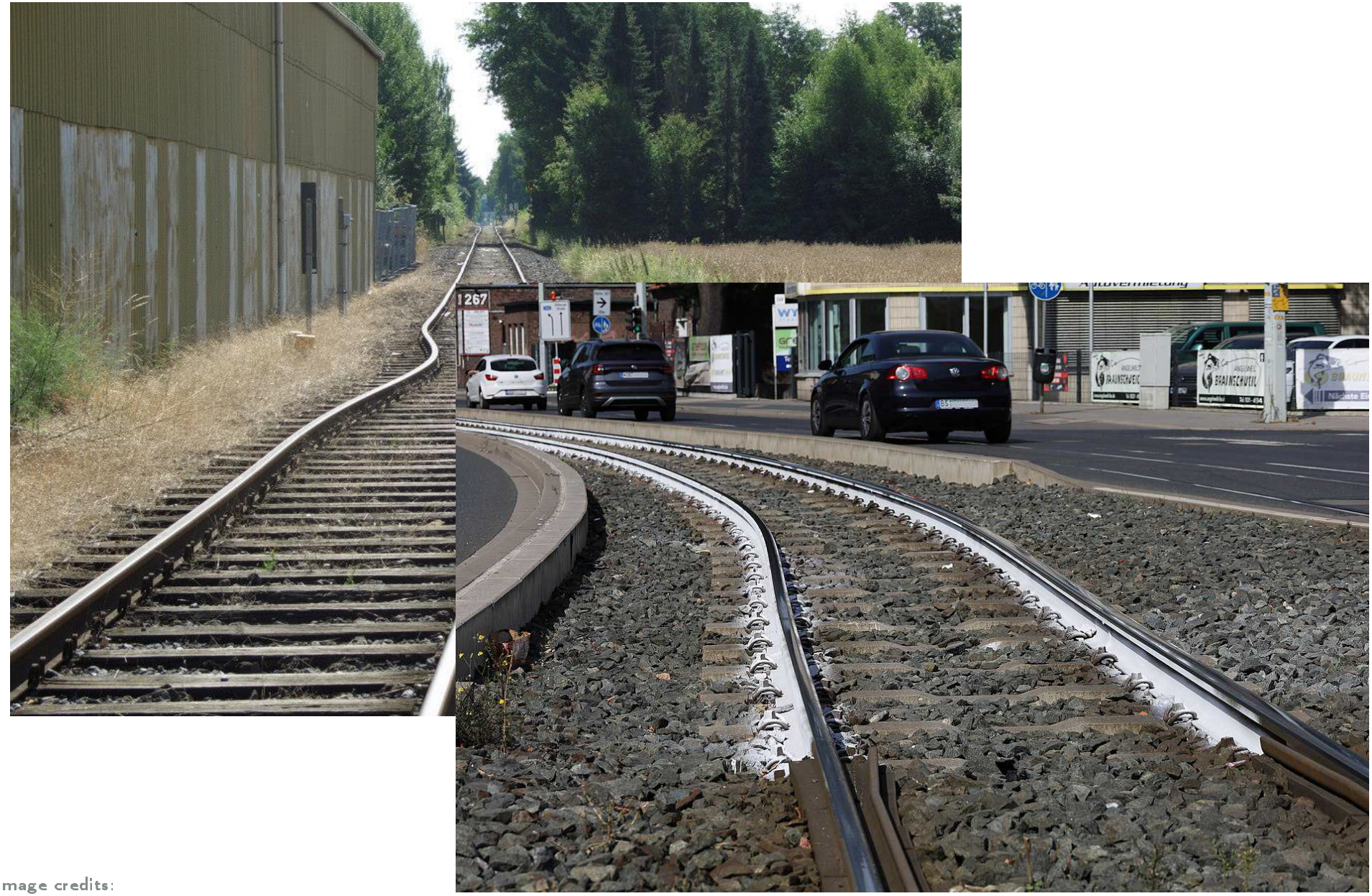
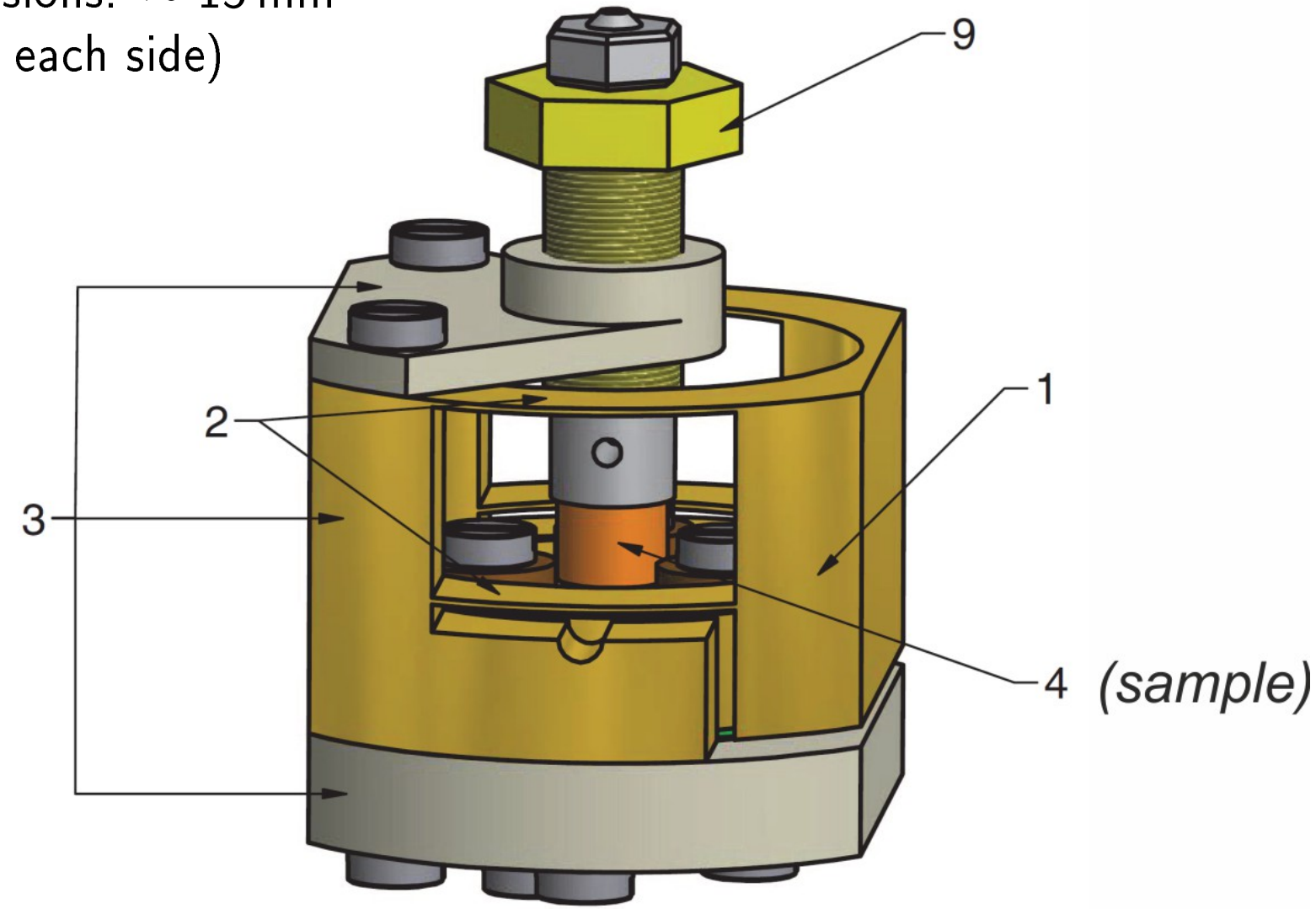


Image credits:
ABproTWE and TeWeBs (CC-BY-SA)

Experimental technique

dilatometry

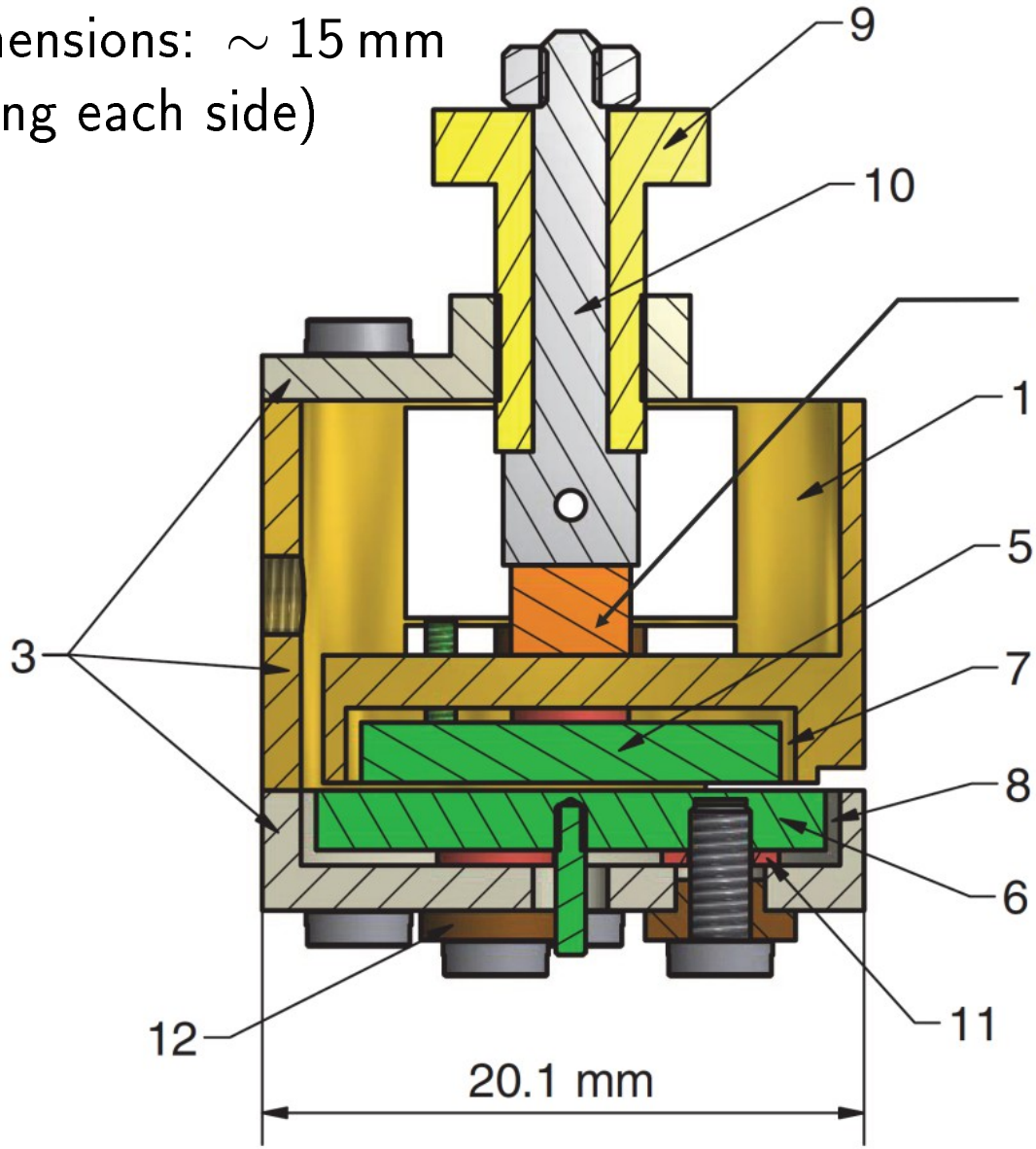
Dimensions: $\sim 15\,\mathrm{mm}$
(along each side)



Rev. Sci. Instrum. 83, 095102 (2012)

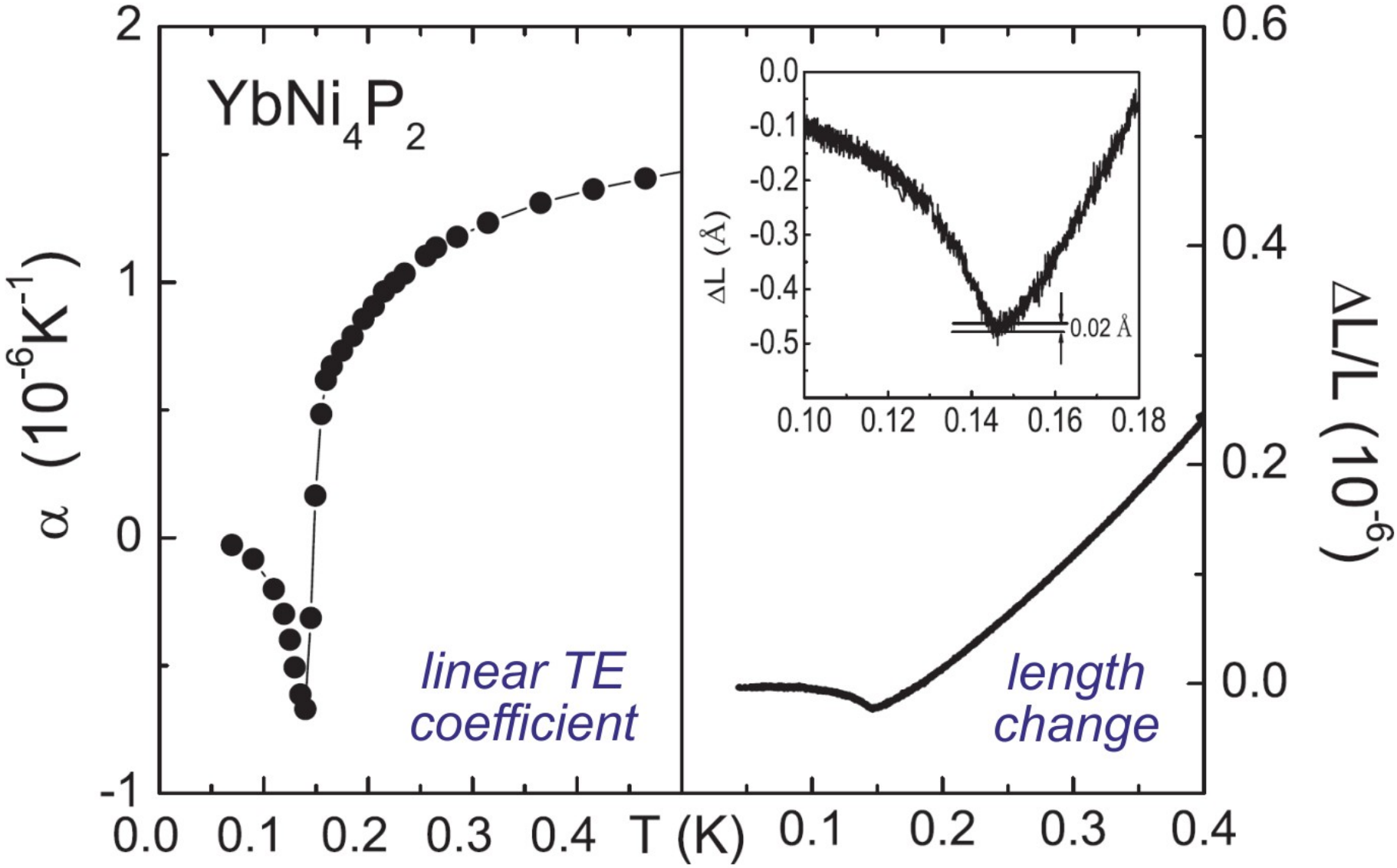
Dimensions: $\sim 15\,\mathrm{mm}$
(along each side)

Resolution in ΔL: 0.02 Å!



Rev. Sci. Instrum. 83, 095102 (2012)

Measurement with a dilatometer



Rev. Sci. Instrum. 83, 095102 (2012)

Sign of α?

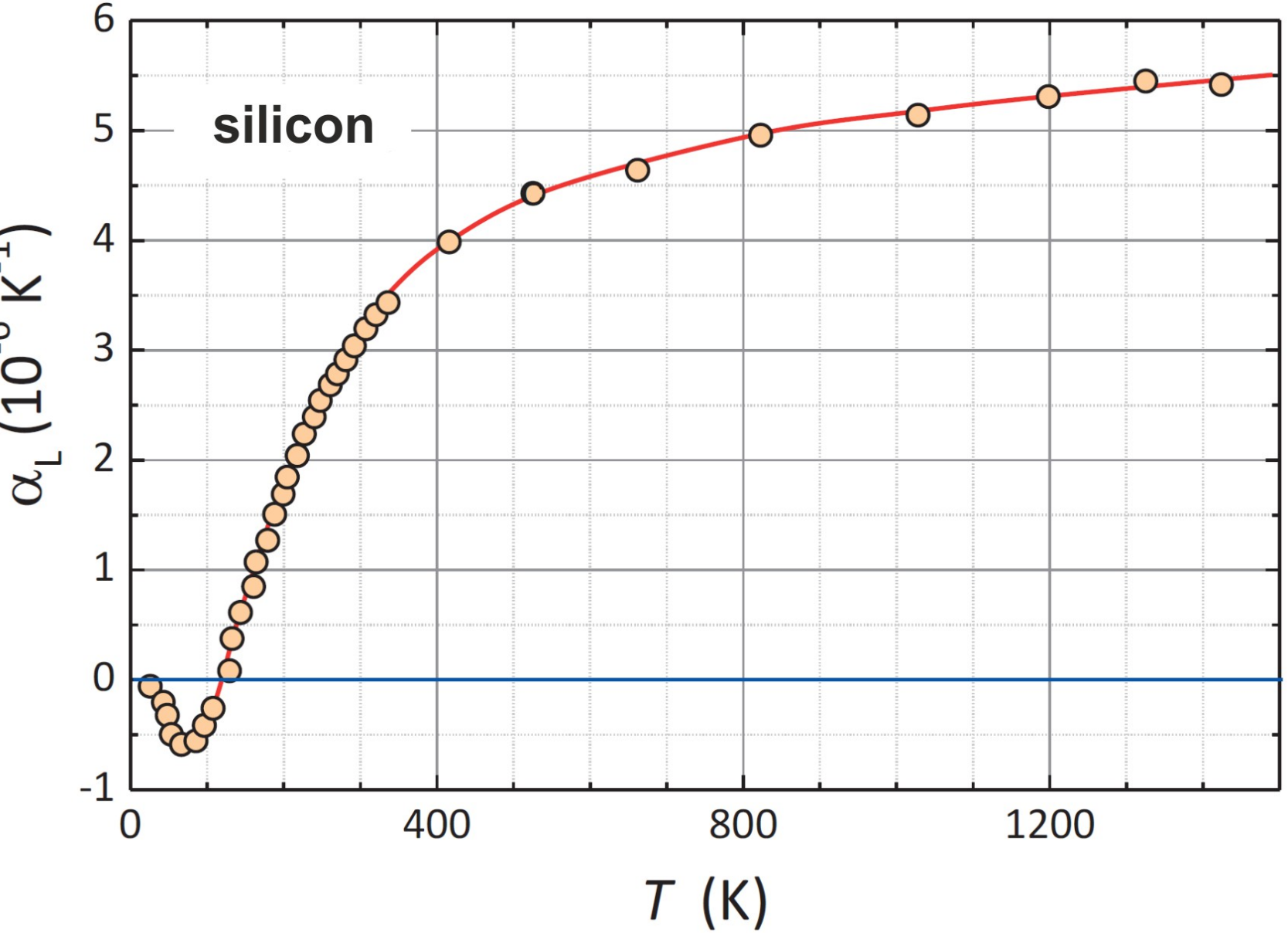


Image credit: S. Hunklinger, Festkörperphysik

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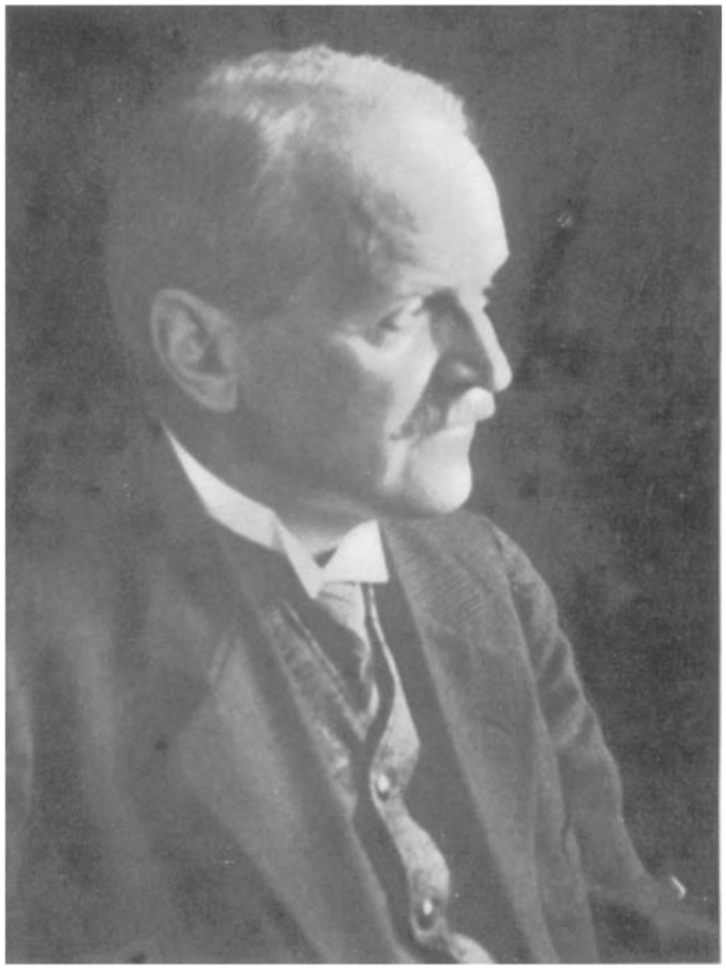
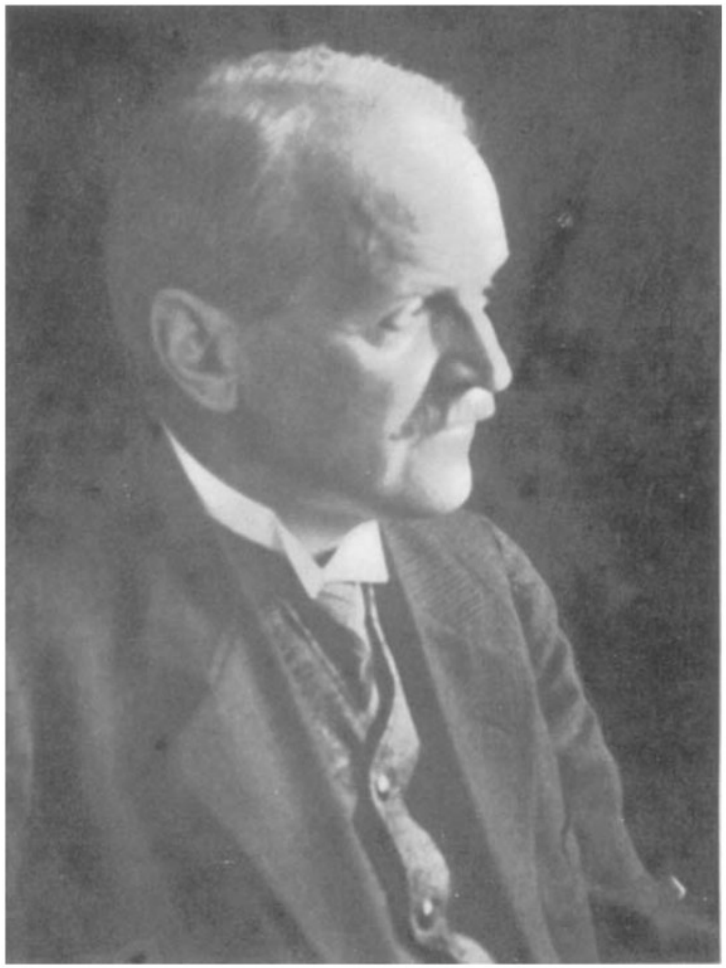
Person

Eduard Grüneisen



Eduard Grüneisen
1877–1949

- 1894–1900: physics studies in Halle and Berlin
- 1900: PhD on electric and thermal conductivities of metals
- 1904–1925: work at *Physikalisch-Technische Reichsanstalt* (Institute of Standards)
- from 1927: professor in Marburg



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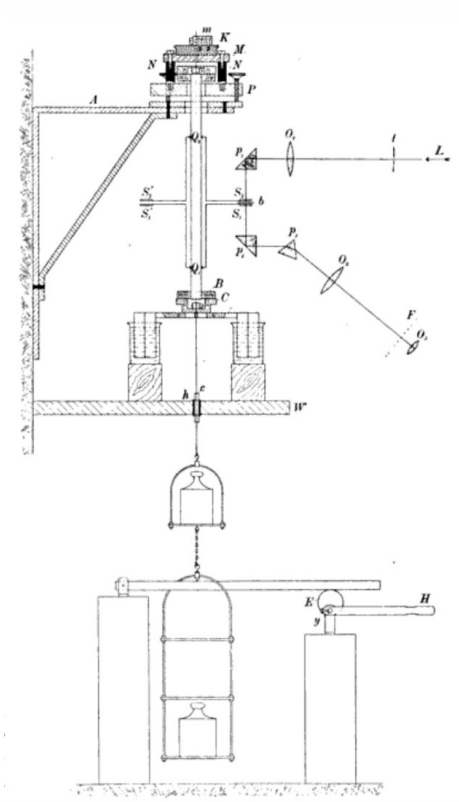
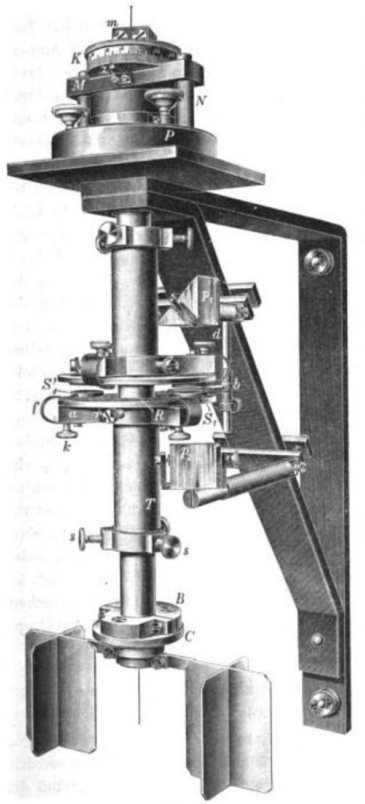




Zeitschrift für Instrumentenkunde 27, 38 (1907)

Thermal expansion vs. heat capacity

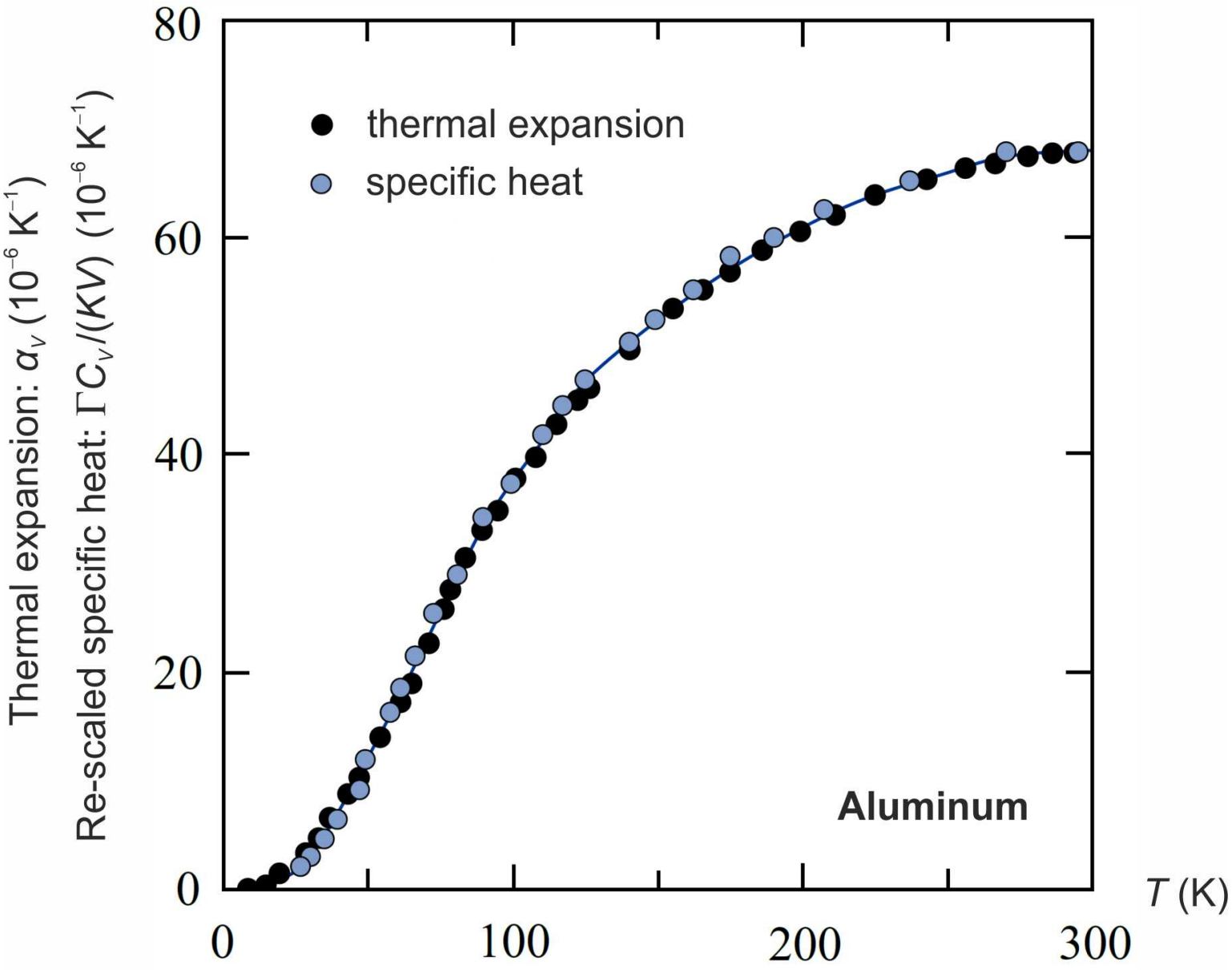
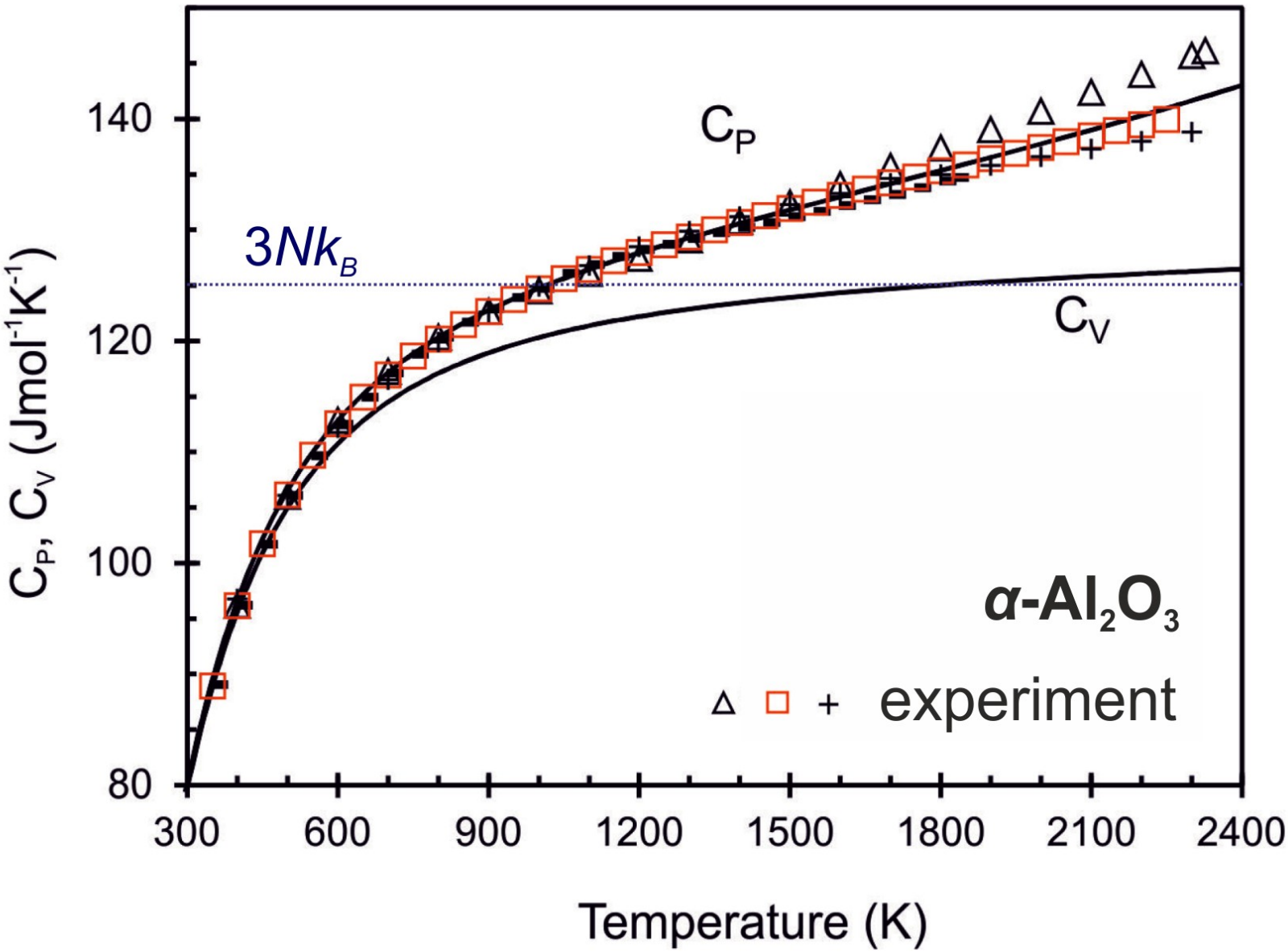
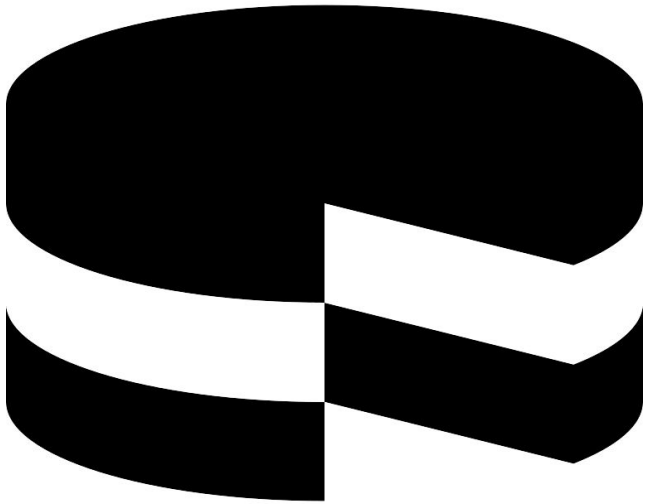


Image credit: S. Hunklinger, Festkörperphysik

Heat capacity: C_p vs. C_V



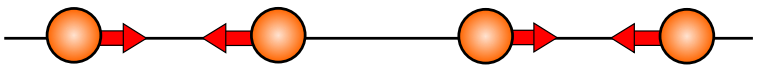
Geodynamics & Tectonophysics 7, 459 (2016)

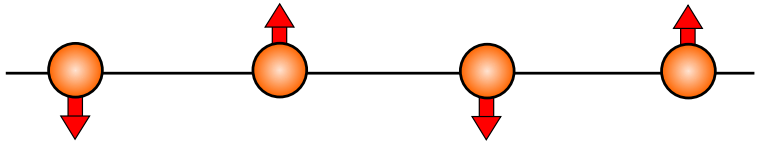


Material

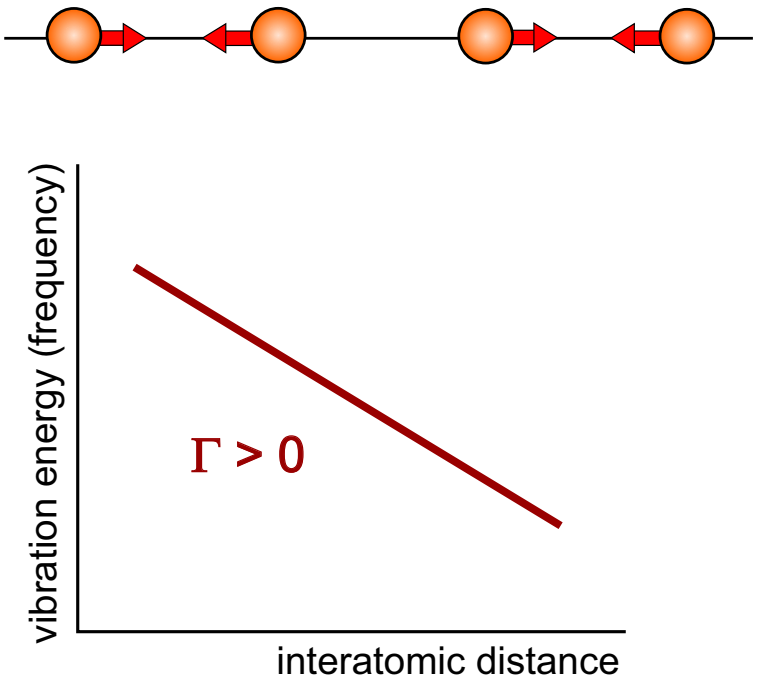
negative thermal expansion (NTE) materials

Longitudinal vs. transverse modes





Longitudinal vs. transverse modes



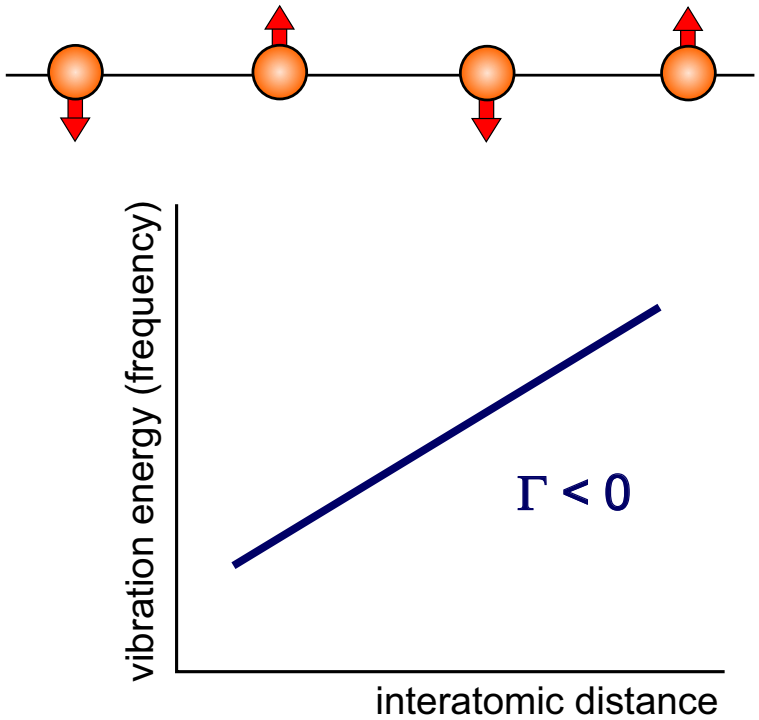
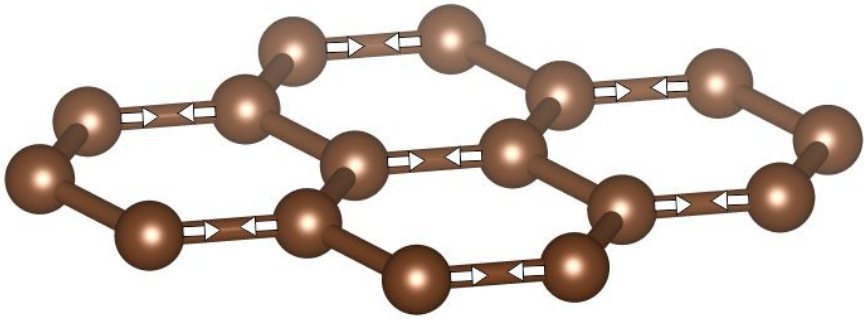
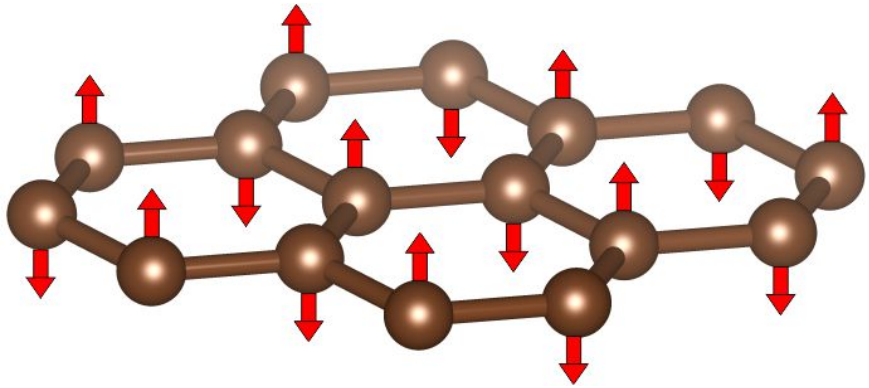


Image credit: Martin Möller (CC-BY-SA)

Example: graphene





High-energy (hard) mode

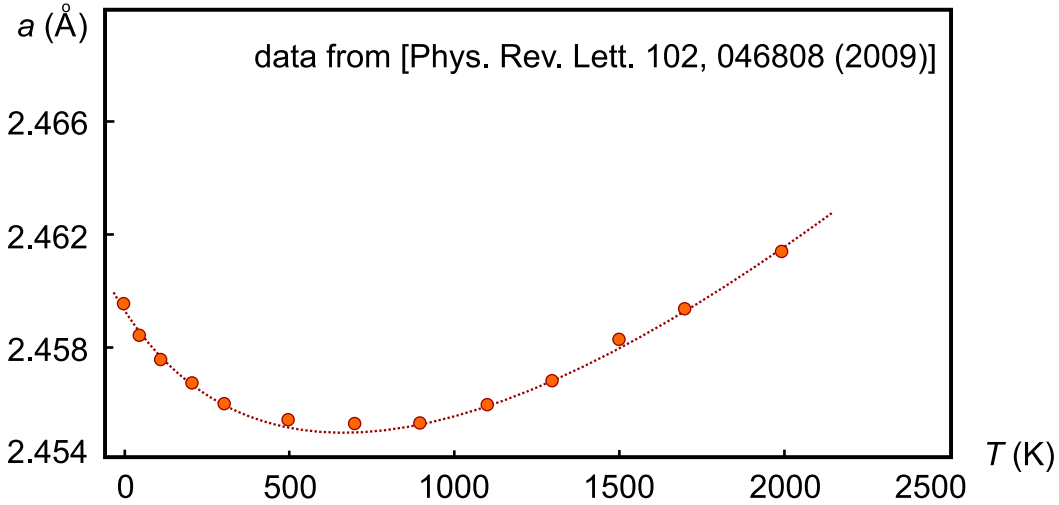
positive thermal expansion,

but only at very high T's

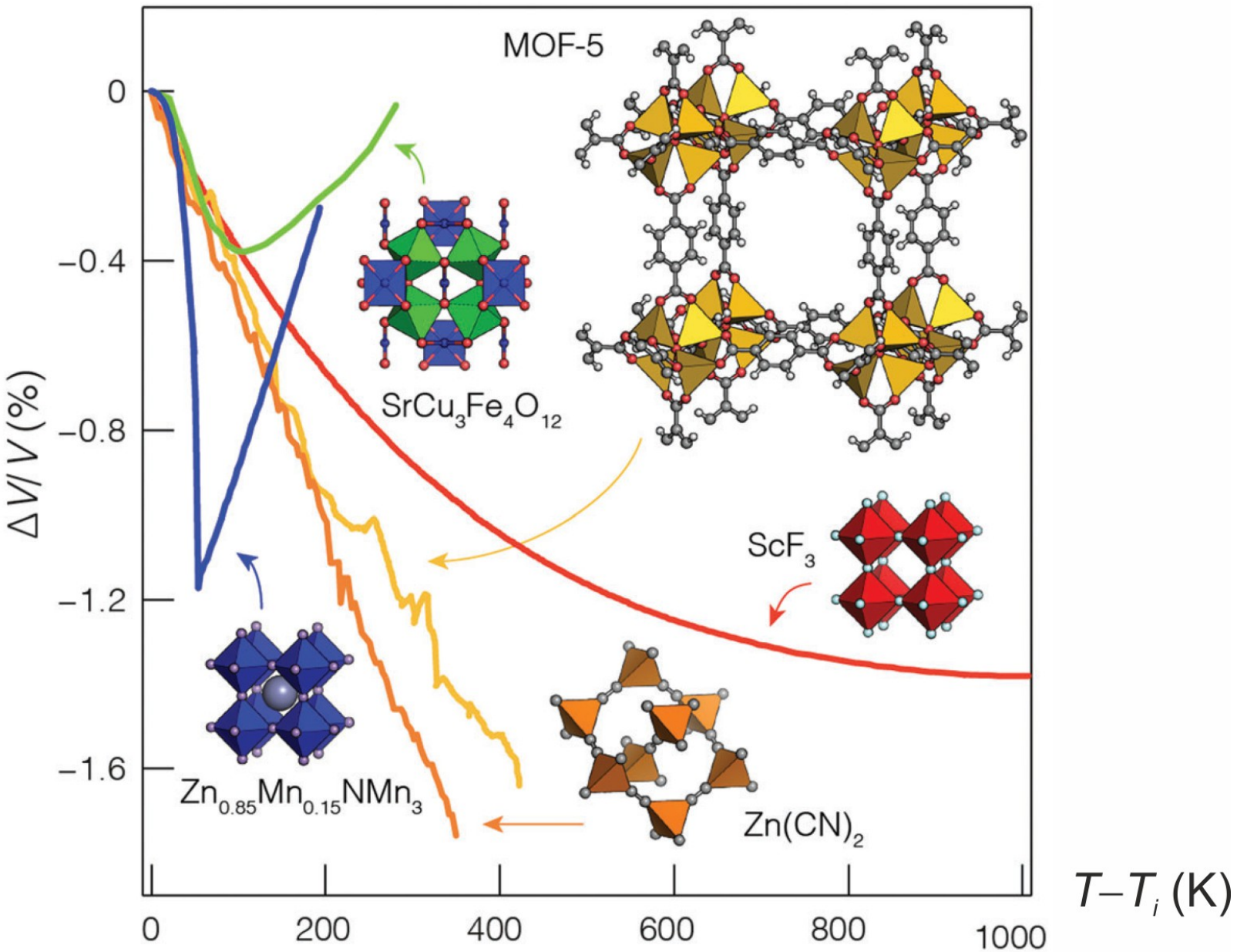
Low-energy (soft) mode

negative thermal expansion

up to $\sim 1000\,\mathrm{K}$

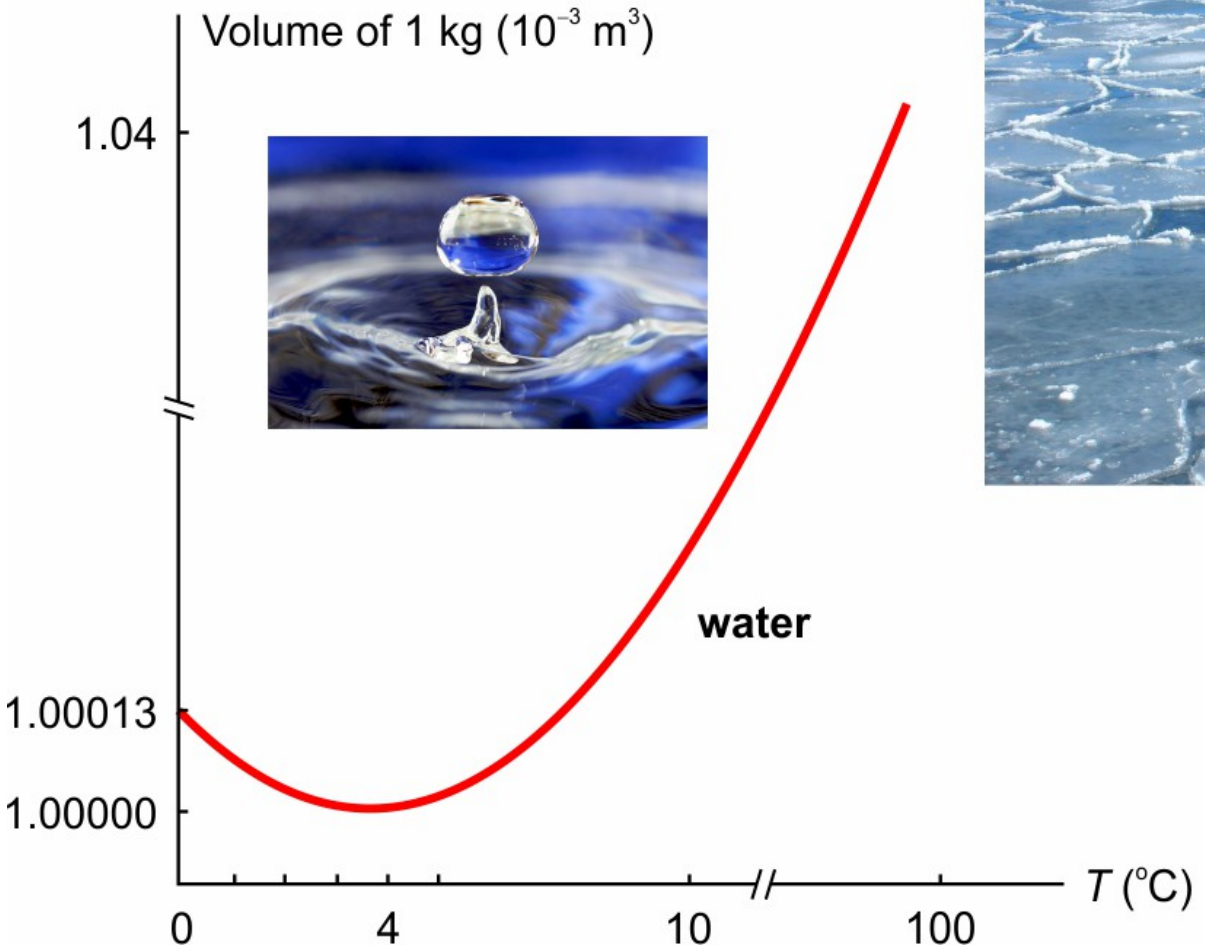


Negative thermal expansion materials



Mater. Horizons 6, 211 (2019)

Implications



Ice floats
on the water

Water at 4 °C
goes to the bottom

Image credits: José Manuel Suárez and Hans Kylberg (CC-BY-SA)

Image credits: Open Clipart and Felix Reimann (CC-BY-SA)