Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin
Nationales Metrologieinstitut

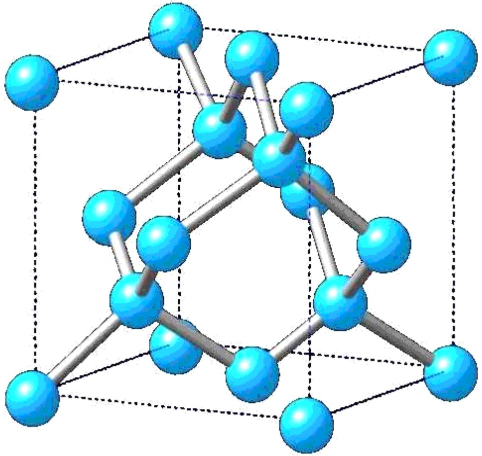
Silicon spheres for the realization of the new kilogram definition

CCM, 17 May 2019

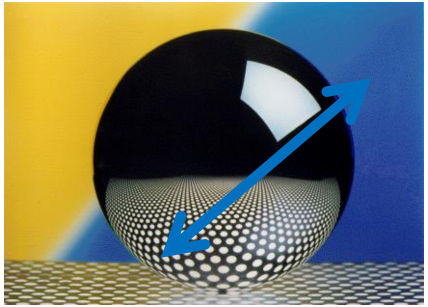
Horst Bettin, PTB Germany

Counting atoms: XRCD method

Use of a silicon crystal!



1. Volume a_0^3 of the unit cell
2. Volume of an atom: $a_0^3/8$
3. Volume *V* of a sphere
4. Number *N* of the atoms



$$N = \frac{V_{\mathrm{Si}}}{v_{\mathrm{Atom}}} = \frac{V_{\mathrm{Si}}}{(a^3/8)}$$

Realization of the mass unit

Mass of the sphere including surface layers:

$$m_{\text{sphere}} = \frac{2\,h\,R_\infty}{c\,\alpha^2} \frac{\sum x(^i\text{Si})\,A_\text{r}(^i\text{Si})}{A_\text{r}(\text{e})} \frac{8\,V_{\text{core}}}{a^3} - m_{\text{deficit}} + m_{\text{SL}}$$

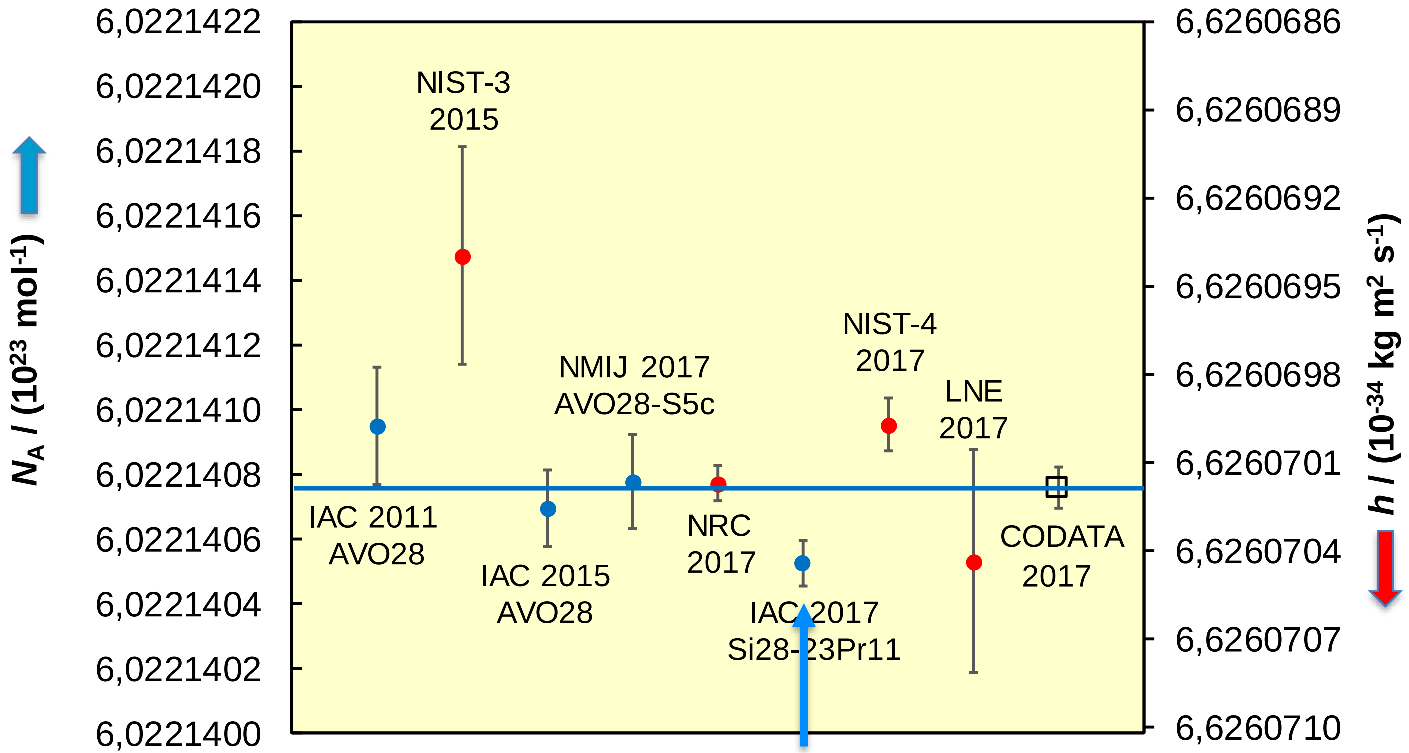
Electron mass	Mean mass ratio	Number of atoms	Point defects	Surface layers

***h*:**	**Planck constant**
R_∞:	**Rydberg constant**
***c*:**	**speed of light in vacuum**
α :	**fine-structure constant**

$x(^i\text{Si})$:	**amount-of-substance ratio of ^{i}Si in the sphere (*i* = 28, 29, 30)**
A_r:	**relative atomic mass**
e:	**electron**
V_{core}:	**volume of the Si-28 sphere without surface layers**
***a*:**	**lattice parameter**
m_{deficit}:	**correction for impurities and vacancies in the sphere**
m_{SL}:	**mass of surface layers**

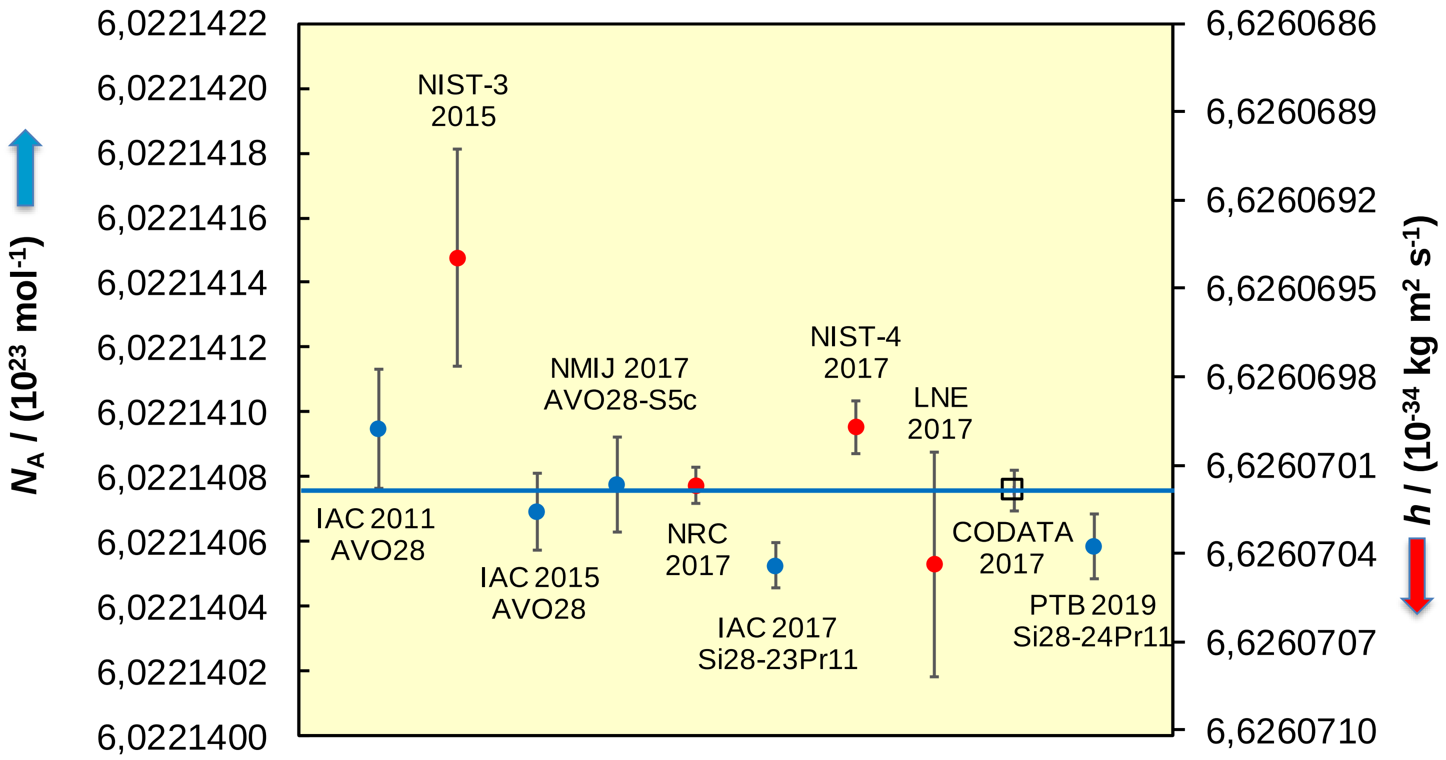
Partners	Lattice parameter		Sphere volume	Sphere mass	Molar mass	Crystal perfection	Surface	Sphere fabrication
	Abs.	Rel.						
BIPM				X			H_2O	
INRIM	X				^{30}Si	X		
ITRI				X			2019?	
METAS							XPS	
NIM			2019?	?	X		X?	?
NIST		?			X			
NMI-A								X
NMIJ		X	X	X	X	X	X	
NRC					X			
PTB	2019?	2019?	X	X	X	X	X	X

CODATA 2017 Special Adjustment



Rel. Unc. 1.2 x 10^{-8}

Si28 crystals



Published uncertainties in 10^{-9}

Quantity	Si28kg01a (NMIJ)	Si28kg01a (PTB)	Si28kg01b (PTB)
Molar mass	1.5	1.5	1.3
Sphere mass	5.9	6.1	6.1
Sphere surface	7.9	7.6	6.0
Sphere volume	19.5	7.0	7.0
Lattice parameter	5.2	5.2	5.2
Point defects	4.7	4.7	6.2
Total uncert. (k = 1)	23.0	14.1	14.0

Advantages of the XRCD experiment

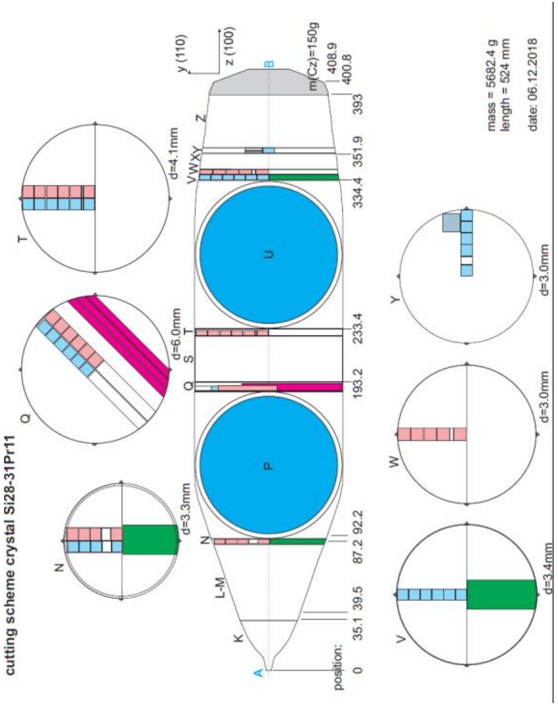
Advantages of the XRCD experiment

- Only the surface layer has to be measured each time in the realizing lab
- Volume measurements every 5 years, e. g. at PTB or NMIJ
- Molar mass, impurities etc. only once
- Si-28 sphere can be purchased
- Surface measurement is “state of the art”, can be set up within about two years.
- Relative uncertainty for the mass unit of about 1×10^{-8}.

Main progress of the XRCD experiment

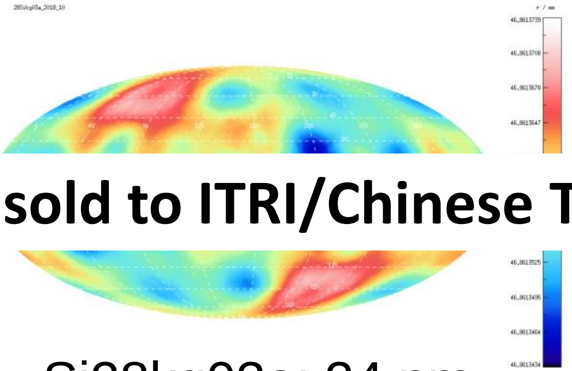
- Third and fourth ^{28}Si single crystals were grown
- One ^{28}Si sphere was sold to ITRI/Chinese Taipei (with the construction details of the XRF/XPS apparatus)

^{28}Si single crystals of PTB



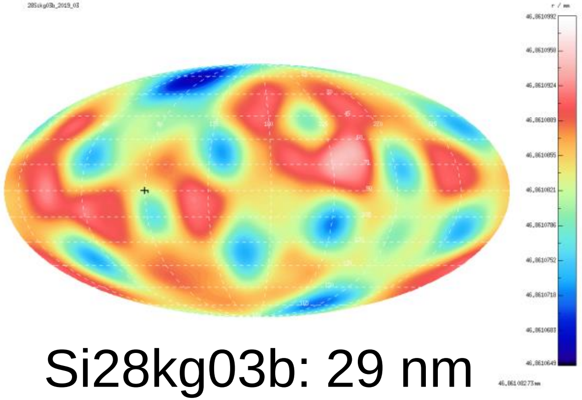
Si28-31Pr11, April 2018

m = 5682 g, 99.9985 % ^{28}Si



sold to ITRI/Chinese Taipei

Si28kg03a: 24 nm



Si28kg03b: 29 nm

Future

Future progress of the XRCD experiment

- Measurements of existing crystals will be completed 2019
- Two more ^{28}Si single crystals (4 spheres) are to come in 2019
- New lattice parameter apparatus at PTB nearly operational
- Project to simulate the carbon concentration distribution in the Si-28 crystals together with the Leibniz-Institute of Crystal Growth (IKZ) in Berlin
- Uncertainty of surface measurements to be improved.

Checks

Relative measurements to check differences between the ^{28}Si crystals:

- **Mass differences**
- **Density differences by the pressure-of-flotation method**
- **Lattice parameter difference measurements are planned**
- **Molar mass difference measurements?**

Natural Silicon spheres

- As secondary mass standards:
  stable, mass can be “reset” by cleaning, sphere can be used as mass standard immediately after cleaning
- Molar mass measurements for natural silicon: uncertainty about 1 ppm, this is sufficient for small samples (below 1 g)
  Precondition: homogeneity of molar mass in small dimensions
- kg realization after density comparison to a Si-28 sphere,
  Si-28 spheres are primary density standards (no volume or mass measurement of the sphere necessary)

Realization of the mass unit

Mass of the sphere including surface layers:

$$m_{\text{sphere}} = \frac{2\,h\,R_\infty}{c\,\alpha^2} \frac{\sum x(^i\text{Si})\,A_r(^i\text{Si})}{A_r(\text{e})} \frac{8\,V_{\text{core}}}{a^3} - m_{\text{deficit}} + m_{\text{SL}}$$

Electron mass	Mean mass ratio	Number of atoms	Point defects	Surface layers

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Realization of the density unit

$$m_{\text{sphere}} = \frac{2\,h\,R_\infty}{c\,\alpha^2}\,\frac{\sum x({}^i\text{Si})\,A_\text{r}({}^i\text{Si})}{A_\text{r}(\text{e})}\,\frac{8\,V_{\text{core}}}{a^3} - m_{\text{deficit}} + m_{\text{SL}}$$

Neglecting surface layers and point defects:

$$m_{\text{sphere}} = \frac{2\,h\,R_\infty}{c\,\alpha^2}\,\frac{\sum x({}^i\text{Si})\,A_\text{r}({}^i\text{Si})}{A_\text{r}(\text{e})}\,\frac{8\,V_{\text{core}}}{a^3}$$

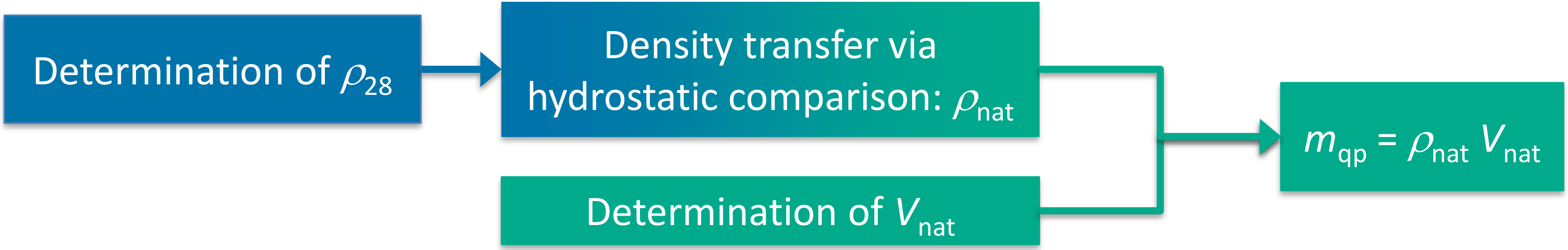
yields the density of the sphere and a direct realisation of the density unit:

$$\rho_{28} = \frac{m_{\text{sphere}}}{V_{\text{core}}} = \frac{2\,h\,R_\infty}{c\,\alpha^2}\,\frac{\sum x({}^i\text{Si})\,A_\text{r}({}^i\text{Si})}{A_\text{r}(\text{e})}\,\frac{8}{a^3}$$

(No mass or volume determination of the sphere is necessary!)

Natural silicon: a less expensive alternative

- By means of a hydrostatic comparison the density of ^{28}Si can be transferred to a ^{nat}Si sphere
  - ➢ Only the density of the **^{28}Si sphere** has to be known
  - ➢ Volume and mass of the **^{28}Si sphere** will **not** be used
- After an accurate determination of the volume of the sphere, the **^{nat}Si sphere** is a primary realisation of the new kg ("quasi-primary")



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Small masses

- Mass of small silicon samples can be determined
  by density and volume measurements:
  $$m = \rho V .$$
  Also for natural silicon!
  Precondition: homogeneity of the density in small dimensions