Crystal Density and Atomic Packing Factor from Lattice Parameter

Theoretical density of a cubic crystal from atoms per unit cell, atomic mass and lattice parameter, and the atomic packing factor from the atomic radius.

Method: Unit cell density and packing

Input parameters

Unit system: SI

Parameter	Value	Unit
Atoms per unit cell (BCC 2, FCC 4)	4.0000	
Atomic mass	63.550	kg/kmol
Lattice parameter	0.36150	nm
Atomic radius (0 to skip APF)	0.12780	nm

Calculated results

Parameter	Value	Unit
Theoretical density	8.9351	g/cm³
Unit cell volume	4.7242e-23	cm³
Atomic packing factor	0.74031	
Atoms per cubic metre	8.4671e+28	

Notes for this case

• ρ = nA/(V_cN_A) with V_c = a³ for cubic cells: n = 1 simple cubic, 2 BCC, 4 FCC (and 8 for diamond cubic). APF = n(4/3)πr³/V_c: 0.52, 0.68 and 0.74 for SC, BCC and FCC with touching atoms (a = 4r/√3 for BCC, 2√2r for FCC). Measured density is a little lower because of vacancies and porosity.

Formula and method

$$\rho = \frac{nA}{V_c N_A}, \quad APF = \frac{n\frac{4}{3}\pi r^3}{V_c}$$

Variables

n	Atoms per unit cell (BCC 2, FCC 4)	-
A	Atomic mass	kg/kmol
a	Lattice parameter	m
r	Atomic radius (0 to skip APF)	m
ρ	Theoretical density	kg/m³
V_c	Unit cell volume	m³
APF	Atomic packing factor	-
n/V_c	Atoms per cubic metre	-

Method and standards

Crystal density.

Assumptions and limits

- Cubic unit cell; perfect crystal.

References

Unit cell density and packing

Report details

Report reference	FCC-TFXB-H6RB (the same inputs always give the same reference)
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Release checks	3 reference cases of this calculator, computed independently, are checked on every release

Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/materials/properties/crystal-density-lattice

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.