Equilibrium Vacancy Concentration in a Metal

Number of atomic sites and equilibrium vacancies per cubic metre from density, atomic mass, vacancy formation energy and temperature.

Method: Equilibrium point-defect statistics

Input parameters

Unit system: SI

Parameter	Value	Unit
Density	8,400.0	kg/m³
Atomic mass	63.500	kg/kmol
Vacancy formation energy	0.90000	eV
Temperature	1,000.0	°C

Calculated results

Parameter	Value	Unit
Atomic sites (per m³)	7.9663e+28	
Vacancies (per m³)	2.1807e+25	
Vacancy site fraction	2.7374e-04	

Notes for this case

• N = N_Aρ/A atomic sites per unit volume; N_v = N·exp(−Q_v/kT). Near the melting point the vacancy fraction reaches about 10^{-4}; at room temperature it is negligible unless vacancies are quenched in. Vacancies control substitutional diffusion, climb and creep. The default is copper at 1,000 °C (density at room temperature).

Formula and method

$$N = \frac{N_A \rho}{A}, \quad N_v = N \exp\left(-\frac{Q_v}{kT}\right)$$

Variables

ρ	Density	kg/m³
A	Atomic mass	kg/kmol
Q_v	Vacancy formation energy	J
T	Temperature	K
N	Atomic sites (per m³)	-
N_v	Vacancies (per m³)	-
N_v/N	Vacancy site fraction	-

Method and standards

Vacancies.

Assumptions and limits

- Equilibrium; isolated vacancies; constant formation energy.

References

Equilibrium point-defect statistics

Report details

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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/vacancy-concentration

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.