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Part 12: Condensed matter physics

Grandeurs et unités —

Partie 12: Physique de la matière condensée

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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Fax: +41 22 749 09 47
Email: copyright@iso.org
Website: www.iso.org

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www. iso. org/directives).

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This document was prepared by Technical Committee ISO/TC 12, *Quantities and units*, in collaboration with Technical Committee IEC/TC 25, *Quantities and units*.

This second edition cancels and replaces the first edition (ISO 80000-12:2009), which has been technically revised.

The main changes compared to the previous edition are as follows:

— the table giving the quantities and units has been simplified;

— some definitions and the remarks have been stated physically more precisely.

A list of all parts in the ISO 80000 and IEC 80000 series can be found on the ISO and IEC websites.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Quantities and units —

Part 12: Condensed matter physics

1 Scope

This document gives names, symbols, definitions and units for quantities of condensed matter physics. Where appropriate, conversion factors are also given.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

Names, symbols, definitions and units for quantities used in condensed matter physics are given in Table 1.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

Table 1 — Quantities and units used in condensed matter physics

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
12-1.1	lattice vector	$\boldsymbol{R}$	translation vector that maps the crystal lattice on itself	m	The non-SI unit ångström (Å) is widely used by x-ray crystallographers and structural chemists.
12-1.2	fundamental lattice vectors	$\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$	fundamental translation vectors for the crystal lattice	m	The lattice vector (item 12-1.1) can be given as $\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$ where n_1, n_2 and n_3 are integers.
12-2.1	angular reciprocal lattice vector	$\boldsymbol{G}$	vector whose scalar products with all fundamental lattice vectors are integral multiples of 2π	m^{-1}	In crystallography, however, the quantity $\frac{\boldsymbol{G}}{2\pi}$ is sometimes used.
12-2.2	fundamental reciprocal lattice vectors	$\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$	fundamental translation vectors for the reciprocal lattice	m^{-1}	$\boldsymbol{a}_i \cdot \boldsymbol{b}_i = 2\pi\delta_{ij}$ In crystallography, however, the quantities $\frac{\boldsymbol{b}_j}{2\pi}$ are also often used.
12-3	lattice plane spacing	d	distance (ISO 80000-3) between successive lattice planes	m	The non-SI unit ångström (Å) is widely used by x-ray crystallographers and structural chemists.
12-4	Bragg angle	ϑ	angle between the scattered ray and the lattice plane	1 °	Bragg angle ϑ is given by $2d \sin\vartheta = n\lambda$ where d is the lattice plane spacing (item 12-3), λ is the wavelength (ISO 80000-7) of the radiation, and n is the order of reflexion which is an integer.
12-5.1	short-range order parameter	r, σ	fraction of nearest-neighbour atom pairs in an Ising ferromagnet having magnetic moments in one direction, minus the fraction having magnetic moments in the opposite direction	1	Similar definitions apply to other order-disorder phenomena. Other symbols are frequently used.
12-5.2	long-range order parameter	R, s	fraction of atoms in an Ising ferromagnet having magnetic moments in one direction, minus the fraction having magnetic moments in the opposite direction	1	Similar definitions apply to other order-disorder phenomena. Other symbols are frequently used.

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
12-5.3	atomic scattering factor	f	quotient of radiation amplitude scattered by the atom and radiation amplitude scattered by a single electron	1	The atomic scattering factor can be expressed by: $f = \frac{E_a}{E_e}$ where E_a is the radiation amplitude scattered by the atom and E_e is the radiation amplitude scattered by a single electron.
12-5.4	structure factor	$F(h,k,l)$	quantity given by: $F(h,k,l) = \sum_{n=1}^{N} f_n \exp[2\pi i(hx_n + ky_n + lz_n)]$ where f_n is the atomic scattering factor (item 12-5.3) for atom n, x_n, y_n, z_n are fractional coordinates of its position, N is the total number of atoms in the unit cell and h, k, l are the Miller indices	1	For the Miller indices h, k, l, see Annex A.
12-6	Burgers vector	$\boldsymbol{b}$	closing vector in a sequence of vectors encircling a dislocation	m	
12-7.1	particle position vector	$\boldsymbol{r}$, $\boldsymbol{R}$	position vector (ISO 80000-3) of a particle	m	Often, $\boldsymbol{r}$ is used for electrons and $\boldsymbol{R}$ is used for atoms and other heavier particles.
12-7.2	equilibrium position vector <condensed matter physics>	$\boldsymbol{R}_0$	position vector (ISO 80000-3) of an ion or atom in equilibrium	m	
12-7.3	displacement vector <condensed matter physics>	$\boldsymbol{u}$	difference between the position vector (ISO 80000-3) of an ion or atom and its position vector in equilibrium	m	The displacement vector can be expressed by: $\boldsymbol{u} = \boldsymbol{R} - \boldsymbol{R}_0$ where $\boldsymbol{R}$ is particle position vector (item 12-7.1) and $\boldsymbol{R}_0$ is position vector of an ion or atom in equilibrium (item 12-7.2).
12-8	Debye-Waller factor	D, B	factor by which the intensity of a diffraction line is reduced because of the lattice vibrations	1	D is sometimes expressed as $D = \exp(-2W)$; in Mössbauer spectroscopy, it is also called the f factor and denoted by f.

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
12-9.1	angular wavenumber, angular repetency <condensed matter physics>	k, (q)	quotient of momentum (ISO 80000-4) and the reduced Planck constant (ISO 80000-1)	m^{-1}	The corresponding vector (ISO 80000-2) quantity is called wave vector (ISO 80000-3), expressed by: $\boldsymbol{k}=\frac{\boldsymbol{p}}{\hbar}$ where $\boldsymbol{p}$ is the momentum (ISO 80000-4) of quasi free electrons in an electron gas, and $\hbar$ is the reduced Planck constant (ISO 80000-1); for phonons, its magnitude is $k=\frac{2\pi}{\lambda}$ where λ is the wavelength (ISO 80000-3) of the lattice vibrations. When a distinction is needed between k and the symbol for the Boltzmann constant (ISO 80000-1), k_B can be used for the latter. When a distinction is needed, q should be used for phonons, and k for particles such as electrons and neutrons. The method of cut-off must be specified. In condensed matter physics, angular wavenumber is often called wavenumber.
12-9.2	Fermi angular wavenumber, Fermi angular repetency	k_F	angular wavenumber (item 12-9.1) of electrons in states on the Fermi sphere	m^{-1}	In condensed matter physics, angular wavenumber is often called wavenumber.
12-9.3	Debye angular wavenumber, Debye angular repetency	q_D	cut-off angular wavenumber (item 12-9.1) in the Debye model of the vibrational spectrum of a solid	m^{-1}	The method of cut-off must be specified. In condensed matter physics, angular wavenumber is often called wavenumber.
12-10	Debye angular frequency	ω_D	cut-off angular frequency (ISO 80000-3) in the Debye model of the vibrational spectrum of a solid	s^{-1}	The method of cut-off must be specified.

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
12-11	Debye temperature	Θ_D	in the Debye model, quantity given by: $\Theta_D = \hbar \frac{\omega_D}{k}$ where k is the Boltzmann constant, (ISO 80000-1), $\hbar$ is the reduced Planck constant (ISO 80000-1), and ω_D is Debye angular frequency (item 12-10)	K	A Debye temperature can also be defined by fitting a Debye model result to a certain quantity, for instance, the heat capacity at a certain temperature.
12-12	density of vibrational states <angular frequency>	g	quotient of the number of vibrational modes in an infinitesimal interval of angular frequency (ISO 80000-3), and the product of the width of that interval and volume (ISO 80000-3)	m^{-3} s	$g(\omega) = n_\omega = \frac{dn(\omega)}{d\omega}$ where $n(\omega)$ is the total number of vibrational modes per volume with angular frequency less than ω. The density of states may also be normalized in other ways instead of with respect to volume. See also item 12-16.
12-13	thermodynamic Grüneisen parameter	γ_G , (Γ_G)	quantity given by: $\gamma_G = \frac{\alpha_V}{\varkappa_T c_V \rho}$ where α_V is cubic expansion coefficient (ISO 80000-5), $\varkappa_T$ is isothermal compressibility (ISO 80000-5), c_V is specific heat capacity at constant volume (ISO 80000-5), and ρ is mass density (ISO 80000-4)	1	
12-14	Grüneisen parameter	γ	quantity given by minus the partial differential quotient: $\gamma = -\frac{\partial \ln \omega}{\partial \ln V}$ where ω is a lattice vibration frequency (ISO 80000-3), and V is volume (ISO 80000-3)	1	ω can also refer to an average of the vibrational spectrum, for instance as represented by a Debye angular frequency (item 12-10).
12-15.1	mean free path of phonons	l_p	average distance (ISO 80000-3) that phonons travel between two successive interactions	m	

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
12-15.2	mean free path of electrons	l_e	average distance (ISO 80000-3) that electrons travel between two successive interactions	m	
12-16	energy density of states	$n_E(E)$, $\rho(E)$	quantity given by the differential quotient with respect to energy: $n_E(E) = \frac{dn(E)}{dE}$ where $n_E(E)$ is the total number of one-electron states per volume (ISO 80000-3) with energy less than E (ISO 80000-5)	$J^{-1}\ m^{-3}$ $eV^{-1}\ m^{-3}$ $kg^{-1}\ m^{-5}\ s^2$	Density of states refers to electrons or other entities, e.g. phonons. It may be normalized in other ways instead of with respect to volume, e.g. with respect to amount of substance. See also item 12-12.
12-17	residual resistivity	ρ_0	for metals, the resistivity (IEC 80000-6) extrapolated to zero thermodynamic temperature (ISO 80000-5)	Ω m $kg\ m^3\ s^{-3}\ A^{-2}$	
12-18	Lorenz coefficient	L	quotient of thermal conductivity (ISO 80000-5), and the product of electric conductivity (IEC 80000-6) and thermodynamic temperature (ISO 80000-3)	V^2/K^2 $kg^2\ m^4\ s^{-6}\ A^{-2}\ K^{-2}$	The Lorenz coefficient can be expressed by $L = \frac{\lambda}{\sigma T}$ where λ is thermal conductivity (ISO 80000-5), σ is electric conductivity (IEC 80000-6), and T is thermodynamic temperature (ISO 80000-5).
12-19	Hall coefficient	R_H, A_H	in an isotropic conductor, relation between electric field strength, $\boldsymbol{E}$, (IEC 80000-6) and electric current density, $\boldsymbol{J}$, (IEC 80000-6) expressed as: $\boldsymbol{E} = \rho \boldsymbol{J} + R_H (\boldsymbol{B} \times \boldsymbol{J})$ where ρ is resistivity (IEC 80000-6), and $\boldsymbol{B}$ is magnetic flux density (IEC 80000-6)	m^3/C $m^3\ s^{-1}\ A^{-1}$	
12-20	thermoelectric voltage (between substances a and b)	E_{ab}	voltage (IEC 80000-6) between substances a and b caused by the thermoelectric effect	V $kg\ m^2\ s^{-3}\ A^{-1}$	

Table 1 *(continued)*

Item No.	Quantity			Unit	Remarks
	Name	Symbol	Definition		
12-21	Seebeck coefficient (for substances a and b)	S_{ab}	differential quotient of thermoelectric voltage with respect to thermodynamic temperature: $S_{ab} = \frac{dE_{ab}}{dT}$ where E_{ab} is the thermoelectric voltage between substances a and b (item 12-20) and T is thermodynamic temperature (ISO 80000-5)	V/K kg m^2 s^{-3} A^{-1} K^{-1}	This term is also called “thermoelectric power”.
12-22	Peltier coefficient (for substances a and b)	Π_{ab}	quotient of Peltier heat power (ISO 80000-5) developed at a junction, and the electric current (IEC 80000-6) flowing from substance a to substance b	V kg m^2 s^{-3} A^{-1}	$\Pi_{ab} = \Pi_a - \Pi_b$ where Π_a and Π_b are the Peltier coefficients of substances a and b, respectively.
12-23	Thomson coefficient	μ	quotient of Thomson heat power (ISO 80000-5) developed, and the electric current (IEC 80000-6) and temperature (ISO 80000-5) difference	V/K kg m^2 s^{-3} A^{-1} K^{-1}	μ is positive if heat is developed when the temperature decreases in the direction of the electric current.
12-24.1	work function	ϕ	difference between energy (ISO 80000-5) of an electron at rest at infinity and the Fermi energy (item 12-27.1)	J eV kg m^2 s^{-2}	The term “energy level” is often used for the state of the electron, not only for its energy. The contact potential difference between substances a and b is given by $V_a - V_b = \frac{\phi_a - \phi_b}{e}$ where e is the elementary charge (ISO 80000-1). A set of energy levels, the energies of which occupy an interval practically continuously, is called an energy band. In semi-conductors E_d and E_a are used for donors and acceptors, respectively.
12-24.2	ionization energy	E_i	difference between energy (ISO 80000-5) of an electron at rest at infinity and a certain energy level which is the energy of an electron in the interior of a substance	J eV kg m^2 s^{-2}	
12-25	electron affinity <condensed matter physics>	χ	energy (ISO 80000-5) difference between an electron at rest at infinity and an electron at the lowest level of the conduction band in an insulator or semiconductor	J eV kg m^2 s^{-2}	