

The Materials Resource Registry is being developed to help researchers find and share materials science resources (collections, repositories, etc.). Thus the materials-related terms used in the system should be most appropriate to describe collections of data instead of individual datasets. Additionally, the terms included here are meant to be used in conjunction with free-text fields that can be populated with terms that are more specific. Examples are listed at the bottom of this document.

This MSE-related vocabulary is intended primarily for use in the Materials Resource Registry being developed at NIST and through the RDA Materials Resource Registry working group, but hopefully it will be applicable to other efforts as well where high-level materials terms are desired.

The first version of this materials vocabulary, used in the application found at matsci.registry.nationaldataservice.org, included categories (e.g., *material type*) and then a single level of selectable values (*metals, polymers, etc.*). However, this was found to be too general to be widely useful to domain experts, even when combined with the free-text keywords. Thus a second level was added to allow for greater specificity while not overwhelming a user with too many checkboxes. In this version of the materials terms, the categories are essentially the same (e.g., *material type*), but an additional level has been added under most of the top-tier terms. An example is *superalloys* under *metals and alloys* in the *materials type* category.

Design constraint: two levels of terms that are as user-friendly and intuitive as possible to describe high-level resources related to materials science data (e.g., repositories or collections)

More than one value can be checked for any category. All categories are optional.

Colors are guides to the eye and show where second-tier terms fit under first-tier terms.

THIS IS A DRAFT AND WILL EVOLVE. It was the major topic for consideration in the 23 Feb 2017 working group meeting in order to set the terms to be used for the remainder of the working group (through Nov 2017).

version 16, 7/13/17

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See below for additional contributors and people/resources consulted

Data origin	experiments
Data origin	informatics and data science
Data origin	simulations

Data origin

theory

Material types	biological	.
Material types	biomaterials	.
Material types	ceramics	.
Material types	ceramics	carbides
Material types	ceramics	cements
Material types	ceramics	nitrides
Material types	ceramics	oxides
Material types	ceramics	perovskites
Material types	ceramics	silicates
Material types	metals and alloys	.
Material types	metals and alloys	Al-containing
Material types	metals and alloys	commercially pure metals
Material types	metals and alloys	Cu-containing
Material types	metals and alloys	Fe-containing
Material types	metals and alloys	intermetallics
Material types	metals and alloys	Mg-containing
Material types	metals and alloys	Ni-containing
Material types	metals and alloys	rare earths
Material types	metals and alloys	refractories
Material types	metals and alloys	steels
Material types	metals and alloys	superalloys
Material types	metals and alloys	Ti-containing
Material types	metamaterials	.
Material types	molecular fluids	.
Material types	organic compounds	.
Material types	organic compounds	<i>alcohols</i>
Material types	organic compounds	<i>aldehydes</i>
Material types	organic compounds	<i>alkanes</i>
Material types	organic compounds	<i>alkenes</i>
Material types	organic compounds	<i>alkynes</i>
Material types	organic compounds	amines
Material types	organic compounds	carboxylic acids
Material types	organic compounds	<i>cyclic compounds</i>

Material types	organic compounds	<i>cycloalkanes</i>
Material types	organic compounds	<i>esters</i>
Material types	organic compounds	<i>ketones</i>
Material types	organic compounds	nitriles
Material types	organometallics	.
Material types	polymers	.
Material types	polymers	copolymers
Material types	polymers	elastomers
Material types	polymers	homopolymers
Material types	polymers	liquid crystals
Material types	polymers	polymer blends
Material types	polymers	rubbers
Material types	polymers	thermoplastics
Material types	polymers	thermosets
Material types	semiconductors	.
Material types	semiconductors	II-VI
Material types	semiconductors	III-V
Material types	semiconductors	extrinsic
Material types	semiconductors	intrinsic
Material types	semiconductors	n-type
Material types	semiconductors	p-type

Structural features	composites	.
Structural features	composites	biological or green
Structural features	composites	fiber-reinforced
Structural features	composites	metal-matrix
Structural features	composites	nanocomposites
Structural features	composites	particle-reinforced
Structural features	composites	polymer-matrix
Structural features	composites	structural
Structural features	defects	.
Structural features	defects	cracks
Structural features	defects	crazing
Structural features	defects	debonding

Structural features	defects	disclinations
Structural features	defects	dislocations
Structural features	defects	inclusions
Structural features	defects	interstitials
Structural features	defects	point defects
Structural features	defects	pores
Structural features	defects	vacancies
Structural features	defects	voids
Structural features	engineered structures	.
Structural features	interfacial	.
Structural features	interfacial	grain boundaries
Structural features	interfacial	interfacial surface area
Structural features	interfacial	interfacial tension or energy
Structural features	interfacial	interfacial thickness
Structural features	interfacial	magnetic domain walls
Structural features	interfacial	ordering boundaries
Structural features	interfacial	phase boundaries
Structural features	interfacial	stacking faults
Structural features	interfacial	surfaces
Structural features	interfacial	twin boundaries
Structural features	microstructures	.
Structural features	microstructures	<i>BCC spheres</i>
Structural features	microstructures	cellular
Structural features	microstructures	clustering
Structural features	microstructures	compound
Structural features	microstructures	crystallinity
Structural features	microstructures	defect structures
Structural features	microstructures	dendritic
Structural features	microstructures	dispersion
Structural features	microstructures	eutectic
Structural features	microstructures	grains
Structural features	microstructures	<i>gyroid</i>
Structural features	microstructures	<i>HEX cylinders</i>
Structural features	microstructures	<i>lamellae</i>
Structural features	microstructures	nanocrystalline

Structural features	microstructures	particle distribution
Structural features	microstructures	particle shape
Structural features	microstructures	polycrystalline
Structural features	microstructures	polydispersity
Structural features	microstructures	porosity
Structural features	microstructures	precipitates
Structural features	microstructures	quasicrystalline
Structural features	microstructures	single crystal
Structural features	microstructures	twinned
Structural features	molecular structure	.
Structural features	molecular structure	alternating copolymer
Structural features	molecular structure	block copolymer
Structural features	molecular structure	<i>bottlebrush</i>
Structural features	molecular structure	dendrimer
Structural features	molecular structure	end-group composition
Structural features	molecular structure	functionalization
Structural features	molecular structure	gradient copolymer
Structural features	molecular structure	long-chain branching
Structural features	molecular structure	<i>molecular weight</i>
Structural features	molecular structure	<i>polydispersity</i>
Structural features	molecular structure	random copolymer
Structural features	molecular structure	short-chain branching
Structural features	molecular structure	surfactants
Structural features	molecular structure	tacticity
Structural features	morphologies	.
Structural features	morphologies	aligned
Structural features	morphologies	amorphous
Structural features	morphologies	<i>anisotropic</i>
Structural features	morphologies	clusters
Structural features	morphologies	complex fluids
Structural features	morphologies	glass
Structural features	morphologies	<i>isotropic</i>
Structural features	morphologies	layered
Structural features	morphologies	nanoparticles or nanotubes
Structural features	morphologies	one-dimensional

Structural features	morphologies	open-framework
Structural features	morphologies	particles or colloids
Structural features	morphologies	<i>percolated</i>
Structural features	morphologies	porous
Structural features	morphologies	quantum dots or wires
Structural features	morphologies	random
Structural features	morphologies	semicrystalline
Structural features	morphologies	thin film
Structural features	morphologies	two-dimensional
Structural features	morphologies	wires
Structural features	morphologies	woven
Structural features	phases	.
Structural features	phases	crystalline
Structural features	phases	disordered
Structural features	phases	gas
Structural features	phases	liquid
Structural features	phases	melt
Structural features	phases	metastable
Structural features	phases	nonequilibrium
Structural features	phases	ordered

Properties addressed	chemical	.
Properties addressed	chemical	composition
Properties addressed	chemical	<i>functional ligands</i>
Properties addressed	chemical	impurity concentration
Properties addressed	chemical	molecular masses and distributions
Properties addressed	chemical	molecular weights
Properties addressed	colligative	.
Properties addressed	corrosion	.
Properties addressed	corrosion	crevice
Properties addressed	corrosion	erosion-corrosion
Properties addressed	corrosion	galvanic
Properties addressed	corrosion	high temperature
Properties addressed	corrosion	intergranular

Properties addressed	corrosion	pitting
Properties addressed	corrosion	selective leaching
Properties addressed	corrosion	stress corrosion
Properties addressed	corrosion	uniform
Properties addressed	crystallographic	.
Properties addressed	crystallographic	crystalline lattice
Properties addressed	crystallographic	orientation maps
Properties addressed	crystallographic	space groups
Properties addressed	crystallographic	textures
Properties addressed	durability	.
Properties addressed	durability	aging
Properties addressed	durability	coefficient of friction
Properties addressed	durability	thermal shock resistance
Properties addressed	durability	water absorption
Properties addressed	durability	wear resistance
Properties addressed	electrical	.
Properties addressed	electrical	band structure
Properties addressed	electrical	conductivity
Properties addressed	electrical	<i>current and energy density</i>
Properties addressed	electrical	<i>dielectric breakdown strength</i>
Properties addressed	electrical	dielectric constant and spectra
Properties addressed	electrical	dielectric dispersion
Properties addressed	electrical	electrostrictive
Properties addressed	electrical	piezoelectric
Properties addressed	electrical	power conversion efficiency
Properties addressed	electrical	pyroelectric
Properties addressed	electrical	resistivity
Properties addressed	electrical	spin polarization
Properties addressed	electrical	superconductivity
Properties addressed	electrical	thermoelectric
Properties addressed	kinetic	.
Properties addressed	kinetic	grain growth
Properties addressed	kinetic	phase evolution
Properties addressed	kinetic	phase transitions and ordering
Properties addressed	magnetic	.

Properties addressed	magnetic	coercivity
Properties addressed	magnetic	Curie temperature
Properties addressed	magnetic	magnetization
Properties addressed	magnetic	permeability
Properties addressed	magnetic	saturation magnetization
Properties addressed	magnetic	susceptibility
Properties addressed	mechanical	.
Properties addressed	mechanical	acoustic emission
Properties addressed	mechanical	<i>bulk modulus</i>
Properties addressed	mechanical	compression response
Properties addressed	mechanical	creep
Properties addressed	mechanical	deformation mechanisms
Properties addressed	mechanical	ductility
Properties addressed	mechanical	elasticity
Properties addressed	mechanical	fatigue
Properties addressed	mechanical	flexural response
Properties addressed	mechanical	fracture behavior
Properties addressed	mechanical	fracture toughness
Properties addressed	mechanical	hardness
Properties addressed	mechanical	impact response
Properties addressed	mechanical	phonon modes
Properties addressed	mechanical	plasticity
Properties addressed	mechanical	Poisson's ratio
Properties addressed	mechanical	shear response
Properties addressed	mechanical	strength
Properties addressed	mechanical	stress-strain behavior
Properties addressed	mechanical	tensile response
Properties addressed	mechanical	tensile strength
Properties addressed	mechanical	viscoelasticity
Properties addressed	mechanical	yield strength
Properties addressed	optical	.
Properties addressed	optical	index of refraction
Properties addressed	optical	luminescence
Properties addressed	optical	photoconductivity
Properties addressed	rheological	.

Properties addressed	rheological	complex modulus
Properties addressed	rheological	<i>monomer friction coefficient</i>
Properties addressed	rheological	viscoelasticity
Properties addressed	rheological	viscosity
Properties addressed	structural	.
Properties addressed	thermodynamic	.
Properties addressed	thermodynamic	calorimetry profile
Properties addressed	thermodynamic	critical temperatures
Properties addressed	thermodynamic	crystallization temperature
Properties addressed	thermodynamic	<i>degradation temperature</i>
Properties addressed	thermodynamic	density
Properties addressed	thermodynamic	glass transition temperature
Properties addressed	thermodynamic	grain boundary energies
Properties addressed	thermodynamic	heat capacity
Properties addressed	thermodynamic	heat of fusion
Properties addressed	thermodynamic	heat of solidification
Properties addressed	thermodynamic	interfacial energies
Properties addressed	thermodynamic	liquid crystal phase transition temperature
Properties addressed	thermodynamic	melting temperature
Properties addressed	thermodynamic	molar volume
Properties addressed	thermodynamic	phase diagram
Properties addressed	thermodynamic	phase stability
Properties addressed	thermodynamic	specific heat
Properties addressed	thermodynamic	superconductivity
Properties addressed	thermodynamic	surface energies
Properties addressed	thermodynamic	thermal conductivity
Properties addressed	thermodynamic	thermal decomposition temperature
Properties addressed	thermodynamic	thermal expansion
Properties addressed	toxicity	.
Properties addressed	transport	.
Properties addressed	transport	diffusivity
Properties addressed	transport	grain boundary diffusivity
Properties addressed	transport	interdiffusion
Properties addressed	transport	intrinsic diffusivity
Properties addressed	transport	mobilities

Properties addressed	transport	surface diffusivity
Properties addressed	transport	tracer diffusivity

Characterization methods	charge distribution	.
Characterization methods	charge distribution	pulsed electroacoustic method
Characterization methods	chromatography	.
Characterization methods	chromatography	critical and supercritical chromatography
Characterization methods	chromatography	gas-phase chromatography
Characterization methods	chromatography	ion chromatography
Characterization methods	chromatography	liquid-phase chromatography
Characterization methods	dilatometry	.
Characterization methods	electrochemical	.
Characterization methods	electrochemical	amperometry
Characterization methods	electrochemical	potentiometry
Characterization methods	electrochemical	voltammetry
Characterization methods	mechanical	.
Characterization methods	mechanical	compression tests
Characterization methods	mechanical	creep tests
Characterization methods	mechanical	dynamic mechanical analysis
Characterization methods	mechanical	<i>fatigue testing</i>
Characterization methods	mechanical	<i>hardness testing</i>
Characterization methods	mechanical	<i>in-situ testing</i>
Characterization methods	mechanical	nanoindentation
Characterization methods	mechanical	shear or torsion tests
Characterization methods	mechanical	tension tests
Characterization methods	mechanical	wear tests
Characterization methods	microscopy	.
Characterization methods	microscopy	analytical electron microscopy
Characterization methods	microscopy	atomic force microscopy
Characterization methods	microscopy	confocal microscopy
Characterization methods	microscopy	electron probe microanalysis
Characterization methods	microscopy	environmental scanning electron microscopy
Characterization methods	microscopy	field emission electron probe

Characterization methods	microscopy	optical microscopy
Characterization methods	microscopy	photoluminescence microscopy
Characterization methods	microscopy	scanning Auger electron microscopy
Characterization methods	microscopy	scanning electron microscopy
Characterization methods	microscopy	scanning Kelvin probe
Characterization methods	microscopy	scanning probe microscopy
Characterization methods	microscopy	scanning tunneling microscopy
Characterization methods	microscopy	transmission electron microscopy
Characterization methods	microscopy	x-ray optical interferometry
Characterization methods	optical	.
Characterization methods	optical	differential refractive index
Characterization methods	optical	dynamic light scattering
Characterization methods	optical	ellipsometry
Characterization methods	optical	fractography
Characterization methods	optical	light scattering
Characterization methods	optical	quasi-elastic light scattering
Characterization methods	osmometry	.
Characterization methods	osmometry	freezing point depression osmometry
Characterization methods	osmometry	membrane osmometry
Characterization methods	osmometry	vapor pressure depression osmometry
Characterization methods	profilometry	.
Characterization methods	scattering and diffraction	.
Characterization methods	scattering and diffraction	electron backscatter diffraction
Characterization methods	scattering and diffraction	neutron [elastic] scattering
Characterization methods	scattering and diffraction	neutron [inelastic] scattering
Characterization methods	scattering and diffraction	small angle x-ray scattering
Characterization methods	scattering and diffraction	small-angle neutron scattering
Characterization methods	scattering and diffraction	synchrotron
Characterization methods	scattering and diffraction	x-ray diffraction
Characterization methods	scattering and diffraction	x-ray reflectivity
Characterization methods	scattering and diffraction	x-ray topography
Characterization methods	scattering and diffraction	XRD grazing incidence
Characterization methods	spectrometry	.
Characterization methods	spectrometry	alpha spectrometry
Characterization methods	spectrometry	energy dispersive x-ray spectrometry

Characterization methods	spectrometry	gamma spectrometry
Characterization methods	spectrometry	ion mobility spectrometry
Characterization methods	spectrometry	IR/FTIR spectrometry
Characterization methods	spectrometry	mass spectrometry
Characterization methods	spectrometry	secondary ion mass spectrometry
Characterization methods	spectrometry	x-ray fluorescence spectrometry
Characterization methods	spectroscopy	.
Characterization methods	spectroscopy	dielectric and impedance spectroscopy
Characterization methods	spectroscopy	dynamic mechanical spectroscopy
Characterization methods	spectroscopy	electron energy-loss spectroscopy
Characterization methods	spectroscopy	EXAFS
Characterization methods	spectroscopy	Fourier-transform infrared spectroscopy
Characterization methods	spectroscopy	<i>neutron spin echo spectroscopy</i>
Characterization methods	spectroscopy	NEXAFS
Characterization methods	spectroscopy	<i>Nuclear Magnetic Resonance</i>
Characterization methods	spectroscopy	<i>Raman spectroscopy</i>
Characterization methods	spectroscopy	x-ray absorption spectroscopy
Characterization methods	spectroscopy	x-ray emission spectroscopy
Characterization methods	spectroscopy	x-ray photoelectron spectroscopy
Characterization methods	spectroscopy	XPS variable kinetic
Characterization methods	thermochemical	.
Characterization methods	thermochemical	calorimetry
Characterization methods	thermochemical	differential scanning calorimetry
Characterization methods	thermochemical	differential thermal analysis
Characterization methods	thermochemical	microcalorimetry
Characterization methods	thermochemical	thermogravimetry
Characterization methods	tomography	.
Characterization methods	tomography	atom probe tomography
Characterization methods	tomography	x-ray tomography
Characterization methods	ultrasonic	.
Characterization methods	viscometry	.

Computational methods boundary tracking or level set

Computational methods	CALPHAD
Computational methods	cellular automata
Computational methods	cluster expansion
Computational methods	crystal plasticity
Computational methods	density functional theory or electronic structure
	<i>discrete element method</i>
Computational methods	dislocation dynamics
	<i>dissipative particle dynamics</i>
Computational methods	finite element analysis
Computational methods	machine learning
Computational methods	<i>micromagnetics simulations</i>
Computational methods	molecular dynamics
Computational methods	Monte Carlo methods
Computational methods	multiscale simulations
Computational methods	phase-field calculations
Computational methods	reverse Monte Carlo
Computational methods	self-consistent field theory
Computational methods	simulated experiment
Computational methods	statistical mechanics

Synthesis and processing	annealing and homogenization	.
Synthesis and processing	annealing and homogenization	aging
Synthesis and processing	annealing and homogenization	<i>dry blending</i>
Synthesis and processing	annealing and homogenization	homogenization
Synthesis and processing	annealing and homogenization	mechanical mixing
Synthesis and processing	annealing and homogenization	melt mixing
Synthesis and processing	annealing and homogenization	normalizing
Synthesis and processing	annealing and homogenization	recrystallization
Synthesis and processing	annealing and homogenization	stress relieving
Synthesis and processing	annealing and homogenization	tempering
Synthesis and processing	annealing and homogenization	<i>twin screw extrusion</i>
Synthesis and processing	annealing and homogenization	ultrasonication
Synthesis and processing	casting	.
Synthesis and processing	casting	centrifugal casting

Synthesis and processing	casting	continuous casting
Synthesis and processing	casting	die casting
Synthesis and processing	casting	investment casting
Synthesis and processing	casting	sand casting
Synthesis and processing	casting	slip casting
Synthesis and processing	casting	vacuum arc melting
Synthesis and processing	deposition and coating	.
Synthesis and processing	deposition and coating	atomic layer deposition
Synthesis and processing	deposition and coating	carbon evaporation coating
Synthesis and processing	deposition and coating	chemical vapor deposition
Synthesis and processing	deposition and coating	electrodeposition
Synthesis and processing	deposition and coating	electron beam deposition
Synthesis and processing	deposition and coating	evaporation
Synthesis and processing	deposition and coating	gold-sputter coating
Synthesis and processing	deposition and coating	ink-jet deposition
Synthesis and processing	deposition and coating	ion beam deposition
Synthesis and processing	deposition and coating	Langmuir-Blodgett film deposition
Synthesis and processing	deposition and coating	physical vapor deposition
Synthesis and processing	deposition and coating	plasma spraying
Synthesis and processing	deposition and coating	pulsed laser deposition
Synthesis and processing	deposition and coating	splatter
Synthesis and processing	deposition and coating	spin coating
Synthesis and processing	deposition and coating	<i>solvent casting</i>
Synthesis and processing	deposition and coating	sputter coating
Synthesis and processing	forming	.
Synthesis and processing	forming	cold rolling
Synthesis and processing	forming	<i>compression molding</i>
Synthesis and processing	forming	drawing
Synthesis and processing	forming	extrusion
Synthesis and processing	forming	forging
Synthesis and processing	forming	hot pressing
Synthesis and processing	forming	hot rolling
Synthesis and processing	forming	injection molding
Synthesis and processing	forming	milling
Synthesis and processing	forming	<i>rotational molding</i>

Synthesis and processing	forming	<i>vacuum molding</i>
Synthesis and processing	forming	<i>molding</i>
Synthesis and processing	fractionation	.
Synthesis and processing	mechanical and surface	.
Synthesis and processing	mechanical and surface	doctor blade or blade coating
Synthesis and processing	mechanical and surface	focused ion beam
Synthesis and processing	mechanical and surface	joining
Synthesis and processing	mechanical and surface	lithography
Synthesis and processing	mechanical and surface	polishing
Synthesis and processing	mechanical and surface	sectioning
Synthesis and processing	mechanical and surface	thermal plasma processing
Synthesis and processing	powder processing	.
Synthesis and processing	powder processing	atomization
Synthesis and processing	powder processing	ball milling
Synthesis and processing	powder processing	centrifugal disintegration
Synthesis and processing	powder processing	hot pressing
Synthesis and processing	powder processing	sintering
Synthesis and processing	powder processing	sponge iron process
Synthesis and processing	quenching	.
Synthesis and processing	quenching	air cooled / quench
Synthesis and processing	quenching	brine quench
Synthesis and processing	quenching	furnace cooled
Synthesis and processing	quenching	gas cooled
Synthesis and processing	quenching	ice quench
Synthesis and processing	quenching	liquid nitrogen quench
Synthesis and processing	quenching	oil quench
Synthesis and processing	quenching	water quench
Synthesis and processing	reactive	.
Synthesis and processing	reactive	addition polymerization
Synthesis and processing	reactive	condensation polymerization
Synthesis and processing	reactive	curing
Synthesis and processing	reactive	dissolving / etching
Synthesis and processing	reactive	drying
Synthesis and processing	reactive	in-situ polymerization
Synthesis and processing	reactive	post-polymerization modification

Synthesis and processing	reactive	reductive roasting
Synthesis and processing	reactive	solution processing
Synthesis and processing	reactive	solvent casting
Synthesis and processing	self-assembly	.
Synthesis and processing	self-assembly	micelle formation
Synthesis and processing	self-assembly	monolayer formation
Synthesis and processing	self-assembly	self-assembly-assisted grafting
Synthesis and processing	solidification	.
Synthesis and processing	solidification	crystallization
Synthesis and processing	solidification	directional solidification
Synthesis and processing	solidification	injection molding
Synthesis and processing	solidification	precipitation
Synthesis and processing	solidification	rapid solidification
Synthesis and processing	solidification	seeded solidification
Synthesis and processing	solidification	single crystal solidification
Synthesis and processing	solidification	vacuum molding
Synthesis and processing	solidification	zone refining

**Sample keywords to include for more specificity
(could be pulled into a controlled vocab for suggestions)**

Heusler phase
ferromagnetic
Li-ion
intermetallics
face-centered cubic
polymer nanocomposite
nucleation
self-assembly
photonic crystal
alumina
topological insulators
Cu-Sn alloys
conventional insulators
metal sulfides
polymorphic transitions

titania slag
ferronickel slags
corrosion

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MRS taxonomy
ASM taxonomy
nanoMine (Richard Zhao)
ThermoML (Erik Pfeif)
Callister, William D., "Materials Science and Engineering: An Introduction,"
5th Edition, Wiley & Sons, New York (2000).

RDA Materials Resource Registry Working Group
CHiMaD "Polymer Data Core" group

Feedback received from

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