Exam questions **14.12.2023**

Crystal structure

1. What is Bravais lattice? Which types of Bravais lattices occur in solids, and how to distinguish between them experimentally?
2. Explain the concept of packing fraction. Elucidate packing fractions for the primitive, body-centered, and face-centered cubic lattices
3. Describe rotation axes as symmetry elements. Which rotation axes are allowed in periodic crystals? What are implications of five-fold symmetry in solids?
4. Explain the difference between the mirror and glide planes. What are experimental fingerprints of the glide planes?
5. Introduce the Neumann's principle and give an example of its application to a tensor property of crystals
6. Explain the phenomenon of chirality. Which symmetry elements are allowed in chiral crystals?
7. Explain the difference between polar and nonpolar crystals. Give examples of the polar and nonpolar point groups.
8. Give an example of a point group of symmetry with at least four elements. List these elements and explain whether this point group is polar or nonpolar and chiral or nonchiral.
9. Explain how atomic positions in crystals are defined. Introduce fractional coordinates and symmetry
10. You work on a new crystal. Which information will you look for in order to visualize and understand its crystal structure?
11. Name at least three crystal systems and explain corresponding symmetries as well as lattice parameters.
12. Explain the phenomenon of dichroism. Which molecules and crystals show strong optical dichroism?
13. Give an example of a space group. Explain the meaning of the symbol.
14. Explain the difference between allotropes, polymorphs, and enantiomorphs. Give one example for each.
15. Introduce the Bragg's law and explain its applications in solid-state physics.
16. What are lattice planes, and how to classify them using Miller indices?
17. What is the structure factor? How can one measure it experimentally?
18. What is reciprocal lattice? Sketch reciprocal-lattice vectors of a hexagonal crystal and indicate their length.
19. Explain the Laue condition and its experimental implications.
20. Explain the concept of Ewald sphere and its implications in scattering experiments.
21. How are lattice planes related to the reciprocal lattice?
22. What is the difference between diffraction experiments on powders and single crystals?
23. Elucidate extinction conditions in a diffraction experiment. Give an example.
24. Explain the difference between elastic and inelastic scattering. Give an example of one experiment of each type and explain which property of a crystal it measures.
25. What is the difference between x-ray and neutron diffraction?

26. You scatter monochromatic x-rays on a crystal. What do you expect to see? How to use this information?

Bonding in crystals, mechanical and dielectric properties

27. Introduce main types of chemical bonds. Give one example of solid for each type of bonding.
28. What is cohesive and lattice energy and how to determine them experimentally?
29. What determines lattice energy of ionic crystals? Explain the meaning of the Madelung constant.
30. Explain the meaning of the ionic radii. How do cation and anion radii influence the structures of ionic crystals? (Pauling's rule).
31. Give at least two examples of close-packed structures of ionic crystals. What determines their stability?
32. What determines lattice energy of van der Waals crystals? Explain changes in the lattice energy of crystals of noble gases.
33. How to elucidate the nature of chemical bonds in a crystal? Which properties should be measured, and what information should be extracted?
34. What is the bulk modulus? How to determine it experimentally?
35. Derive an equation of state for solids, $p = p(V)$ (at constant temperature).
36. Introduce stress and strain and explain their relation. What is the difference between compressive, tensile, and shear strain?
37. What are elastic constants? How to determine them experimentally?
38. Explain the meaning of Poisson's ratio. Give examples of materials with positive, zero, and negative Poisson's ratio.
39. Sketch the stress-strain curve of a solid. Indicate the regions of the elastic and plastic deformation. What is the difference between ductile and brittle materials?
40. Introduce permittivity and polarizability. What is the meaning of complex permittivity?
41. Introduce local electric field in a dielectric. Explain the meaning of depolarizing and Lorentz fields.
42. Sketch real and imaginary parts of the permittivity obtained in the Debye model of relaxation. Give an example of a material that this model can be applied to.
43. Explain operation principle of the microwave oven.

Phonons, thermal properties

44. What is phonon? Explain the difference between acoustic and optical phonons.
45. Sketch phonon dispersion relation for a monoatomic chain. Indicate sound velocity.
46. Compare compressional and shear waves. How do they propagate in solids and liquids?
47. Sketch phonon dispersion for a diatomic chain comprising two atoms with the different mass.
48. Show atomic displacements that correspond to the acoustic and optical phonons in a diatomic chain at $q = 0$ and $q = \pi/a$.

49. Explain the splitting between the transverse and longitudinal optical phonons at $q \simeq 0$ (LO-TO splitting). What does it signal?
50. Introduce the refractive index and elucidate the physical meaning of its real and imaginary parts.
51. Elucidate interaction of light with an optical phonon. What makes ionic crystals reflect light?
52. How to study phonons experimentally? Compare and contrast different techniques.
53. Explain the principle of inelastic x-ray/neutron scattering. What determines the q-range accessible in this experiment?
54. Explain the principle of Brillouin light scattering. Which phonons can be probed?
55. What are the Stokes and anti-Stokes lines? How do they change with temperature?
56. Sketch frequency-dependent permittivity of an ionic crystal with permanent dipoles.
57. Introduce the concept of Brillouin zones. Sketch phonon bands within the first Brillouin zone and explain the notation.
58. What is heat capacity? Sketch heat capacity of a solid as a function of temperature.
59. How to measure heat capacity?
60. Compare Debye and Einstein models of the heat capacity.
61. Explain assumptions of the Debye model (of the heat capacity) and the meaning of the Debye temperature. Elucidate the low-temperature and high-temperature limits.
62. Define thermal expansion. Why do crystals expand upon heating?
63. Introduce the Grüneisen parameter (Γ). What sign of Γ would you expect for longitudinal and transverse phonon modes?
64. Explain the origin of negative thermal expansion.
65. Explain the difference between heat capacities measured at constant volume (c_V) and constant pressure (c_p).
66. Sketch temperature dependence of the crystal volume and of the thermal expansion coefficient.
67. Explain the difference between harmonic and anharmonic approximations in the context of heat capacity, thermal expansion, and thermal conductivity
68. What is thermal conductivity and thermal diffusivity?
69. How to measure thermal conductivity?
70. Sketch temperature dependence of thermal conductivity (lattice contribution). Explain the trends.

Metals, electronic properties

71. What are the main assumptions of the Drude model? Discuss their applicability in the context of real crystals.
72. Derive Drude's expression for the electrical conductivity.

73. How to determine electron concentration in a metal? Why do electron concentrations vary across different metals?
74. Explain the difference between electrical resistivity and resistance. How to measure electrical resistivity?
75. What is the relation between electrical and thermal conductivities of a metal?
76. Elucidate the Wiedemann-Franz law within the Drude and Drude-Sommerfeld models.
77. Explain the Seebeck and Peltier effects.
78. Derive energy levels of electrons in the Fermi gas. What is the Fermi energy?
79. What is density of states? Sketch density of states for the Fermi gas in 1D, 2D, and 3D.
80. Elucidate electronic contribution to the specific heat. Which information can be extracted from the Sommerfeld coefficient?
81. What are Bloch waves and energy bands?
82. Sketch band structure of a simple metal (primitive cubic structure) in the empty-lattice approximation
83. How to map out energy bands experimentally?
84. How is density of states related to the band dispersion? What are van Hove singularities?
85. What is the microscopic difference between metals and insulators?
86. What is the difference between half-metals and semi-metals?
87. How are bad metals different from simple metals?
88. Explain the relation between optical conductivity, permittivity, and refractive index.
89. Sketch optical conductivity of the Drude metal.
90. Explain why metals reflect light. What is plasma frequency?
91. Explain the difference between the intraband and interband contributions to the optical conductivity.
92. What is electron velocity in metals? How is it related to the crystal momentum?
93. What is inertial effective mass of electrons? Show sample band dispersions that cause positive and negative effective mass, respectively.
94. Introduce the Hall effect (in a Drude metal). What information can be extracted from measuring Hall resistivity?
95. Explain tight-binding representation of the band energy. What is the hopping parameter?
96. Sketch band dispersion for a 2D metal (square lattice of atoms) with hoppings restricted to nearest neighbors.
97. What are Wannier functions?
98. What is electron mobility? Give examples of materials with the high mobility.
99. What is the Fermi surface? How to measure it experimentally?
100. Introduce semiclassical model of electron transport and explain (qualitatively) its implications for the electrical conductivity of a metal.

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101. How magnetic field affects electrons in metals?
102. What is cyclotron effective mass?
103. Explain the formation of Landau levels and the origin of quantum oscillations in metals.
104. What are preconditions for the observation of quantum oscillations, and what information can be extracted from their measurement?
105. Sketch temperature dependence of electrical resistivity and elucidate different regimes.