140A-Introduction to Solid State Physics--Study guide for final examination:

Coverage:

Don't worry about memorizing complicated formulas, just try to understand their origin and how to use them. The exam will have a table of pertinent equations and constants on its first page. If needed, I will hand out a sheet with the 14 Bravais lattices.

Reading- See assignments at beginning of each lecture slide set

Some concepts to understand or questions to be able to answer:

•Course introduction:

- How is solid state physics/condensed matter physics important in fundamental science (e.g. Nobel Prizes in Physics, nanoscience) and modern technology (e.g. Moore's Law, magnetic data storage, energy production)?
- What is a field effect transistor? Why is it important?
- What is a nanostructure? Why are they important?

•Review of some basic quantum mechanics and atomic physics: (Largely from Ibach and Luth, but see Appendices A.1-A.3, A.5 in Omar if needed)

- Review of the hydrogen atom problem in quantum mechanics; separation into radial, polar, and azimuthal parts of wave function ψ; extension to many-electron atoms via a screened Coulomb interaction and Z_{eff}
- Conversion of imaginary atomic wave functions into real form for use in linear combination of atomic orbitals (LCAO) = tight-binding (TB) description of covalent bonding
- Many-electron wave functions for Fermions, anti-symmetry and the Pauli Principle
- Anti-symmetry and the Fermi hole for spin-parallel electrons, giving rise to the exchange interaction and lower energies if more electrons have parallel spin, thus also magnetism and Hund's First Rule.
- Filling of the periodic table, including reasoning for order of filling subshells: 1s, 2s, 2p, 3s, 3p, 4s, 3d,…, and special cases when outer d or f shells are half-, or totally-filled

•Bonding in molecules and solids: (Largely Ibach and Luth, but see Omar, Appendices A.7, and A.8 if needed)

•Cohesive energy (lattice energy) of a crystal: meaning and calculation, including from individual bond energies in covalent solids

•Covalent bonding:

- Simple quantum-mechanical description of bonding in a diatomic molecule via LCAO (tight-binding) description, minimization of energy, meaning of H_{AA}, H_{BB}, H_{AB}, H_{BA}, S_{AA}, $S_{BB,}$ $S_{AB,}$ $S_{BA,}$ origin of secular equation for solution
- For simple molecules: bonding and anti-bonding wave functions, sigma and pi character
- Filling of molecular electronic levels
- Energy as a function of interatomic distance for molecules and solids: contributions from electron-nuclear attraction, nuclear-nuclear repulsion, and electron-electron repulsion
- Directed bonds: sp^3 tetrahedral bonding, sp^2+p bonding, other possibilities with d orbitals
- Broadening of electronic states into bands for solids, filling of bands and solid types based on filling: metallic, ferromagnetic metallic, insulator, semiconductor, ionic solid

•Metallic bonding:

- Some valence electrons acting essentially like free electrons, delocalize to reduce their energy and screen the core-core repulsions left behind
- Transition metals (3d, 4d, 5d and 4f, 5f series) have mixture of covalent and metallic bonding, example of Cu $3d^{10}$(covalent)$4s^1$(metallic, free-electron like)

•Ionic bonding:

- Ionization potential and electron affinity
- Electronegativity as measure of net electron attracting power
- Calculation of the net ionic attraction with 1/r variation and the Madelung constant
- Repulsive potential at short distance due to electron-electron repulsion with $1/r^n$ variation
- Calculation of binding energy (lattice energy) of crystal; derivation of pertinent parameters from form of overall interaction

•Van der Waals attraction:

- Oscillating dipoles due to electrons on atoms: $1/r^6$ variation (See supplemental reading from Kittel)

•Hydrogen bonding:

  - H atom bound to very electronegative atom→weak bond to another electronegative atom
- Relative strengths of five interaction types: covalent, metallic, ionic, van der Waals, hydrogen bonding
  - Bloch functions for electrons in periodic potential, general properties
  - Types of solids, recognizable by band structure, densities of state, bandgaps

•Crystal structures: Primarily from Omar, Chapter 1

- Translational periodicity and translation symmetry operations: meaning
- Basis vectors and the Bravais lattice
- Bravais lattice + basis = crystal
- Recognition of the bravais lattice and the basis in a real crystal
- Unit cells: primitive and non-primitive
- Primitive and non-primitive basis vectors for a given structure
- 14 types of three dimensional Bravais lattices
- Planes in crystals and Miller indices: (hkl) and sets {hkl}
- Directions in crystals: [hkl] and sets <hkl>.
- Spacings between planes in crystals with orthogonal basis vectors
- Formulas of compounds from the crystal structure; counting atoms in the unit cell
- Packing of touching spheres in different crystals
- Other special crystal structures: sodium chloride, cesium chloride, diamond
- Calculation of ideal ionic radii ratios in different ionic crystals: cesium chloride, sodium chloride, zinc blende
- Point group symmetry operations: <u>covered lightly</u>
  - Rotations by $2\pi/n$ = n-fold rotation
  - Reflection in a mirror plane
  - Inversion ($\vec{r} \to -\vec{r}$)
- Crystal group = Translation group + Point group

•Diffraction and Crystal Structure Determinations: Primarily from Omar Chapter 2

- Types of scattering and diffracting de Broglie waves: photon, electron, neutron, helium atom,…
- Generation of x-rays: x-ray tube, synchrotron radiation
- Bragg's Law: two views via planar reflection and scattering from an array of individual atoms
- Derivation of the scattered intensity, basic formulas, division into atomic scattering factor f_a, geometric (unit cell or basis) structure factor F and lattice structure factor S
- The atomic scattering factor; general form and derivation
- The reciprocal lattice $G_{hk\ell}$ and the calculation of its basis vectors <u>from the primitive-cell lattice vectors</u> of the real-space lattice
- The Ewald construction to determine allowed reflections
- Forbidden reflections for some crystal structures (e.g., bcc and fcc) due to F
- Fundamental properties of the reciprocal lattice: planar spacings, perpendicularity to planes
- Brillouin zones
- Construction and meaning of the first Brillouin zone (for phonon and electron states, see below)
- Experimental methods of diffraction: powder, Laue
- Diffraction of x-rays, electrons, neutrons-experimental considerations
- Scattering from liquids, Fourier transformation, and the pair function distribution function g(r)
- Scattering from free atoms, Fourier transformation, and the charge density distribution function $\rho(r)$
- The Debye-Waller factor: attenuation of diffraction peaks due to vibrational motion (See supplementary reading from Kittel)

•Lattice vibrations: thermal and acoustic properties: Primarily from Omar, Chapter 3

- Elastic waves in a macroscopic medium, travelling wave solutions, relationship to density and Young's modulus
- Phase and group velocities, velocity of sound
- Counting of states, densities of states
- Basic assumptions of microscopic motion: quantized harmonic oscillator
- Equation of motion and solutions for 1D linear atomic chain: monatomic and diatomic
- Types of vibrations (LA, TA, LO, TO), physical meaning, no. of modes, relative energies
- Phonon densities of states in Brillouin zone, $g(\omega)$; allowed and unallowed ω values
- Relationship between $\omega(q)$ *and* $g(\omega)$; Van Hove singularities, general form in 3D
- Meaning of special points in Brillouin zone
- Gaps and Bragg reflection at zone boundaries; traveling vs. standing waves
- Phonon curves for real materials

- Density of states for isotropic elastic vibrating medium; use in Debye model
- Einstein, Debye, and "exact" models of phonon heat capacity; low-T ($\propto T^3$) and high-T (→3R) limits
- Debye model, meaning of Debye cutoff frequency, Debye temperature
- The phonon: basic properties
- Thermal conductivity as motion of phonons, relaxation time (See supplementary reading from Kittel)
- Inelastic x-ray scattering as Doppler-shifted scattering

•Free electrons in solids: Primarily from Omar Chapter 4

- Basic Schroedinger equation, wave functions, and energy levels
- Counting of states and density of states $g(E) \propto E^{1/2}$
- Fermi-Dirac statistics and F(E)
- Relationship between *E(k)* in Brillouin zone and *g(E);* van Hove singularities
- Fermi sphere, Fermi energy, Fermi wave vector and velocity,
- Internal energy and electronic heat capacity
- Low-T limit of free-electron heat capacity ($\propto T$)
- Electrical conductivity: classical description, drift and random velocities, relaxation time

•Nearly free-electrons in solids: Primarily from Omar Chapter 5, but also drawn from Ibach and Luth Chapter 6

- Basic form of crystal potential and Schrödinger equation in Fourier series representation with *G's*
- Bloch's Theorem, including derivation in periodic potential (Ibach and Luth) and meaning
- Gaps and Bragg reflection at zone boundaries; traveling vs. standing waves; on-potential-well and between potential-well states at zone boundaries with gaps
- Densities of states $\propto 1/(dE/dk)$ and group velocities for real solids that are very free-electron-like (e.g. Al)

•The tight-binding model in solids: Primarily from Omar, Chapter 5, but also drawn from Ibach and Luth Chapter 7

- Recasting of LCAO-MO method into periodic Bloch form
- Neglect of all but nearest-neighbor interactions, as well as overlap between orbitals on adjacent sites
- Splitting of potential into on-site (v) and nearest-neighbor (V') terms
- Basic sinusoidal form of energies, with two key interaction integrals through V': β (single orbital) and interaction/bonding integrals γ (between nearest-neighbor orbitals)
- Analogies to LCAO-MO interaction integrals
- Densities of states $\propto 1/(dE/dk)$ and group velocities for tight-binding and more complex wave functions
- Interpretation of various band structures in terms of the two limiting models above

•Band structure determinations from angle-resolved photoelectron spectroscopy = photoemission (ARPES): Ibach and Luth, Chapter 7, Panel V

- The photoelectric effect revisited, with energy conservation E_{kin}(outside) = $h\nu - E_{binding}$ – (Work function) and k selection rule: $k^f = k^i + G$
- Example measured band structures and relationship to theoretical calculations