PHY455
Spring, 2020
Exam #3

Name _____

Total _____

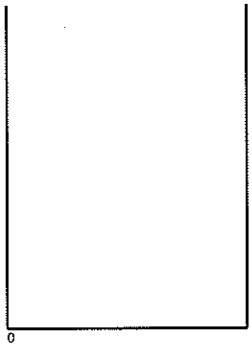
All answers should be given in eV or Å and related units where appropriate, and SI unless otherwise specified. All answers should be given numerically wherever possible unless otherwise stated.

Show your work.

Exam3S20

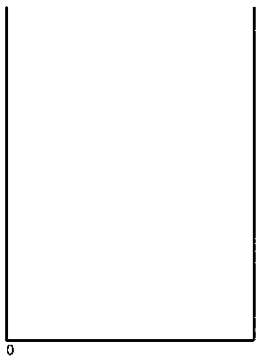
1. a. For a 1D triatomic lattice, evenly spaced atoms, lattice constant a (a/3 between atoms); force constant C, masses M_1, M_2, and M_3. Assume in the nth unit cell the atoms are described by positions u_n, v_n, and w_n. Set up the appropriate equations you would need to find the frequency as a function of k and get it down to a determinant but don't solve it. (**20**)

b. Sketch the phonon dispersion in the 1st BZ. (**10**)



2. A beam of neutrons of wavelength 5.00 Å is incident normally on a cube face (call this the x-direction) of a monoatomic SCC crystal (lattice constant 3.50 Å). Some neutrons are scattered in a single phonon event and exit along the diagonal of the y-z face of the cube with wavelength 4.00 Å. Find the energy (eV) and momentum (SI units) of the phonon involved in this process. (**20**)

3. a. For the 1D case in the Debye Model, find and plot the density of states. (**15**)



b. Find the Debye frequency in terms of atomic density and the velocity of sound. (**10**)

4. For a velocity of sound in lead of 1158 m/s, find the force constant. (**10**)

5. Calculate Plank distribution for 1000K given a frequency of 10^{14} rad/s^{-1}. (**10**)

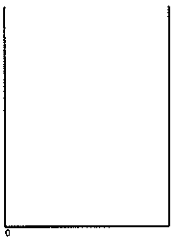
6. a. Find Debye frequency and temperature for germanium. Assume a velocity of sound of 5400 m/s. Compare the Debye temperature to the experimental value. (**10**)

b. For 1 mole of atoms, find the thermal conductivity at 100 K ("high T limit") and compare to experiment (for "normal" germanium-see Figure). (**10**)

7. Assume that $k = B\omega^{\frac{3}{2}} for\ w \leq w_o$

$= 0\ for\ w > w_o$

Find the density of states for the 2D case and plot it. Find ω_o. (**20**)



8. For an ideal monatomic gas at STP (standard temperature and pressure) find the Debye frequency and temperature. Use 319 m/s as the velocity of sound (corresponding to argon). (**10**)

9. Given the dispersion of Na in the [100] direction (Figure 11), estimate a. the force constant from the zone boundary data and b. the velocity of sound from the low frequency data. (**20**) Note: be careful of the units on the plot.

10. For 1 mole of atoms, find the specific heat of K at high T in the Debye model. (**10**)

Table 4 Density and atomic concentration

The data are given at atmospheric pressure and room temperature, or at the stated temperature in deg K. (Crystal modifications as for Table 3.)

H 4K 0.088																	He 2K 0.205 (at 37 atm)
Li 78K 0.542 4.700 3.023	Be 1.82 12.1 2.22											B 2.47 13.0	C 3.516 17.6 1.54	N 20K 1.03	O	F 1.44	Ne 4K 1.51 4.36 3.16
Na 5K 1.013 2.652 3.659	Mg 1.74 4.30 3.20	← Density in g cm^{-3} (10^3kg m^{-3}) →										Al 2.70 6.02 2.86	Si 2.33 5.00 2.35	P	S	Cl 93K 2.03 2.02	Ar 4K 1.77 2.66 3.76
K 5K 0.910 1.402 4.525	Ca 1.53 2.30 3.95	Sc 2.99 4.27 3.25	Ti 4.51 5.66 2.89	V 6.09 7.22 2.62	Cr 7.19 8.33 2.50	Mn 7.47 8.18 2.24	Fe 7.87 8.50 2.48	Co 8.9 8.97 2.50	Ni 8.91 9.14 2.49	Cu 8.93 8.45 2.56	Zn 7.13 6.55 2.66	Ga 5.91 5.10 2.44	Ge 5.32 4.42 2.45	As 5.77 4.65 3.16	Se 4.81 3.67 2.32	Br 123K 4.05 2.36	Kr 4K 3.09 2.17 4.00
Rb 5K 1.629 1.148 4.837	Sr 2.58 1.78 4.30	Y 4.48 3.02 3.55	Zr 6.51 4.29 3.17	Nb 8.58 5.56 2.86	Mo 10.22 6.42 2.72	Tc 11.50 7.04 2.71	Ru 12.36 7.36 2.65	Rh 12.42 7.26 2.69	Pd 12.00 6.80 2.75	Ag 10.50 5.85 2.89	Cd 8.65 4.64 2.98	In 7.29 3.83 3.25	Sn 5.76 2.91 2.81	Sb 6.69 3.31 2.91	Te 6.25 2.94 2.86	I 4.95 2.36 3.54	Xe 4K 3.78 1.64 4.34
Cs 5K 1.997 0.905 5.235	Ba 3.59 1.60 4.35	La 6.17 2.70 3.73	Hf 13.20 4.52 3.13	Ta 16.66 5.55 2.86	W 19.25 6.30 2.74	Re 21.03 6.80 2.74	Os 22.58 7.14 2.68	Ir 22.55 7.06 2.71	Pt 21.47 6.62 2.77	Au 19.28 5.90 2.88	Hg 227 14.26 4.26 3.01	Tl 11.87 3.50 3.46	Pb 11.34 3.30 3.50	Bi 9.80 2.82 3.07	Po 9.31 2.67 3.34	At —	Rn —
Fr —	Ra —	Ac 10.07 2.66 3.76															

Ce 6.77 2.91 3.65	Pr 6.78 2.92 3.63	Nd 7.00 2.93 3.66	Pm —	Sm 7.54 3.03 3.59	Eu 5.25 2.04 3.96	Gd 7.89 3.02 3.58	Tb 8.27 3.22 3.52	Dy 8.53 3.17 3.51	Ho 8.80 3.22 3.49	Er 9.04 3.26 3.47	Tm 9.32 3.32 3.54	Yb 6.97 3.02 3.88	Lu 9.84 3.39 3.43
Th 11.72 3.04 3.60	Pa 15.37 4.01 3.21	U 19.05 4.80 2.75	Np 20.45 5.20 2.62	Pu 19.81 4.26 3.1	Am 11.87 2.96 3.61	Cm —	Bk —	Cf —	Es —	Fm —	Md —	No —	Lr —

Periodic Table of the Elements

Group I	Group II	Transition elements									Group III	Group IV	Group V	Group VI	Group VII	Group 0
H 1 1.007 9 1s																He 2 4.002 6 1s²
Li 3 6.941 2s¹	Be 4 9.0122 2s²										B 5 10.811 2p¹	C 6 12.011 2p²	N 7 14.007 2p³	O 8 15.999 2p⁴	F 9 18.998 2p⁵	Ne 10 20.180 2p⁶
Na 11 22.990 3s¹	Mg 12 24.305 3s²										Al 13 26.982 3p¹	Si 14 28.086 3p²	P 15 30.974 3p³	S 16 32.066 3p⁴	Cl 17 35.453 3p⁵	Ar 18 39.948 3p⁶
K 19 39.098 4s¹	Ca 20 40.078 4s²	Sc 21 44.956 3d¹4s²	Ti 22 47.867 3d²4s²	V 23 50.942 3d³4s²	Cr 24 51.996 3d⁵4s¹	Mn 25 54.938 3d⁵4s²	Fe 26 55.845 3d⁶4s²	Co 27 58.933 3d⁷4s²	Ni 28 58.693 3d⁸4s²	Cu 29 63.546 3d¹⁰4s¹	Zn 30 65.41 3d¹⁰4s²	Ga 31 69.723 4p¹	Ge 32 72.64 4p²	As 33 74.922 4p³	Se 34 78.96 4p⁴	Br 35 79.904 4p⁵	Kr 36 83.80 4p⁶
Rb 37 85.468 5s¹	Sr 38 87.62 5s²	Y 39 88.906 4d¹5s²	Zr 40 91.224 4d²5s²	Nb 41 92.906 4d⁴5s¹	Mo 42 95.94 4d⁵5s¹	Tc 43 (98) 4d⁵5s²	Ru 44 101.07 4d⁷5s¹	Rh 45 102.91 4d⁸5s¹	Pd 46 106.42 4d¹⁰	Ag 47 107.87 4d¹⁰5s¹	Cd 48 112.41 4d¹⁰5s²	In 49 114.82 5p¹	Sn 50 118.71 5p²	Sb 51 121.76 5p³	Te 52 127.60 5p⁴	I 53 126.90 5p⁵	Xe 54 131.29 5p⁶
Cs 55 132.91 6s¹	Ba 56 137.33 6s²	57–71*	Hf 72 178.49 5d²6s²	Ta 73 180.95 5d³6s²	W 74 183.84 5d⁴6s²	Re 75 186.21 5d⁵6s²	Os 76 190.23 5d⁶6s²	Ir 77 192.2 5d⁷6s²	Pt 78 195.08 5d⁹6s¹	Au 79 196.97 5d¹⁰6s¹	Hg 80 200.59 5d¹⁰6s²	Tl 81 204.38 6p¹	Pb 82 207.2 6p²	Bi 83 208.98 6p³	Po 84 (209) 6p⁴	At 85 (210) 6p⁵	Rn 86 (222) 6p⁶
Fr 87 (223) 7s¹	Ra 88 (226) 7s²	89–103**	Rf 104 (261) 6d²7s²	Db 105 (262) 6d³7s²	Sg 106 (266)	Bh 107 (264)	Hs 108 (277)	Mt 109 (268)	Ds 110 (271)	Rg 111 (272)	Cn 112 (285)	113†† (284)	Fl 114 (289)	115†† (288)	Lv 116 (293)	117†† (294)	118†† (294)

Symbol — Ca 20 — Atomic number
Atomic mass† — 40.078
4s² — Electron configuration

*Lanthanide series	La 57 138.91 5d¹6s²	Ce 58 140.12 5d¹4f¹6s²	Pr 59 140.91 4f³6s²	Nd 60 144.24 4f⁴6s²	Pm 61 (145) 4f⁵6s²	Sm 62 150.36 4f⁶6s²	Eu 63 151.96 4f⁷6s²	Gd 64 157.25 4f⁷5d¹6s²	Tb 65 158.93 4f⁹6s²	Dy 66 162.50 4f¹⁰6s²	Ho 67 164.93 4f¹¹6s²	Er 68 167.26 4f¹²6s²	Tm 69 168.93 4f¹³6s²	Yb 70 173.04 4f¹⁴6s²	Lu 71 174.97 4f¹⁴5d¹6s²
**Actinide series	Ac 89 (227) 6d¹7s²	Th 90 232.04 6d²7s²	Pa 91 231.04 5f²6d¹7s²	U 92 238.03 5f³6d¹7s²	Np 93 (237) 5f⁴6d¹7s²	Pu 94 (244) 5f⁶7s²	Am 95 (243) 5f⁷7s²	Cm 96 (247) 5f⁷6d¹7s²	Bk 97 (247) 5f⁹6d¹7s²	Cf 98 (251) 5f¹⁰7s²	Es 99 (252) 5f¹¹7s²	Fm 100 (257) 5f¹²7s²	Md 101 (258) 5f¹³7s²	No 102 (259) 5f¹⁴7s²	Lr 103 (262) 5f¹⁴6d¹7s²

Note: Atomic mass values given are averaged over isotopes in the percentages in which they exist in nature.
† For an unstable element, mass number of the most stable known isotope is given in parentheses.

††Elements 113, 115, 117, and 118 have not yet been officially named. Only small numbers of atoms of these elements have been observed.
Note: For a description of the atomic data, visit *physics.nist.gov/PhysRefData/Elements/per_text.html*.

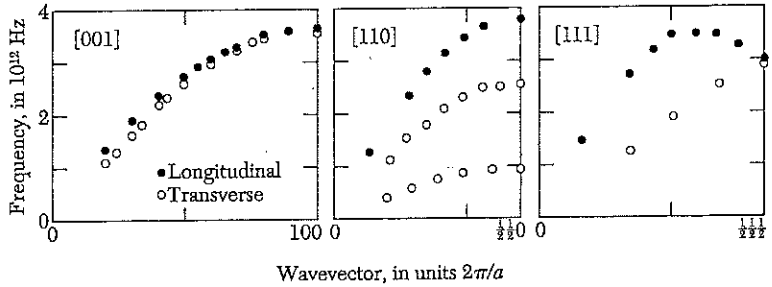


Figure 11 The dispersion curves of sodium for phonons propagating in the [001], [110], and [111] directions at 90 K, as determined by inelastic scattering of neutrons, by Woods, Brockhouse, March and Bowers.

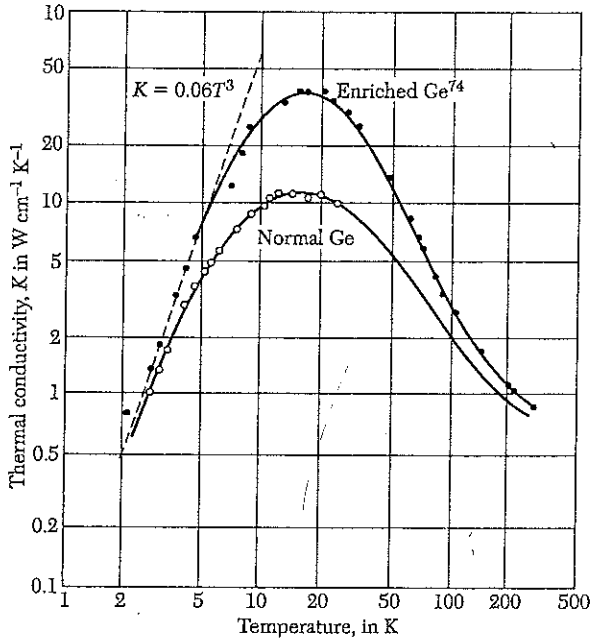


Table 1 Debye temperature and thermal conductivity[a]

Low-temperature limit of θ, in Kelvin
Thermal conductivity at 300 K, in W $cm^{-1}K^{-1}$

Li	Be											B	C	N	O	F	Ne
344 0.85	1440 2.00											0.27	2230 1.29				75
Na	Mg											Al	Si	P	S	Cl	Ar
158 1.41	400 1.56											428 2.37	645 1.48				92
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
91 1.02	230	360 0.16	420 0.22	380 0.31	630 0.94	410 0.08	470 0.80	445 1.00	450 0.91	343 4.01	327 1.16	320 0.41	374 0.60	282 0.50	90 0.02		72
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn w	Sb	Te	I	Xe
56 0.58	147	280 0.17	291 0.23	275 0.54	450 1.38	0.51	600 1.17	480 1.50	274 0.72	225 4.29	209 0.97	108 0.82	200 0.67	211 0.24	153 0.02		64
Cs	Ba	La β	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
38 0.36	110	142 0.14	252 0.23	240 0.58	400 1.74	430 0.48	500 0.88	420 1.47	240 0.72	165 3.17	71.9	78.5 0.46	105 0.35	119 0.08			
Fr	Ra	Ac															

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
0.11	0.12	0.16		0.13		200 0.11	0.11	210 0.11	0.16	0.14	0.17	120 0.35	210 0.16
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
163 0.54		207 0.28	0.06	0.07									