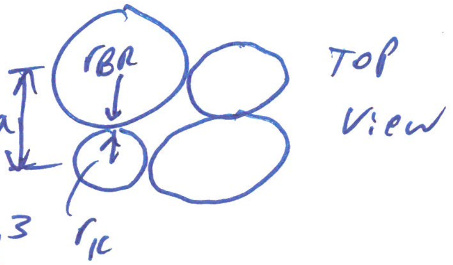
EE 362 Electronic, Magnetic, & Optical Properties of Materials
Examination #1 (Spring 2024)

Name Key

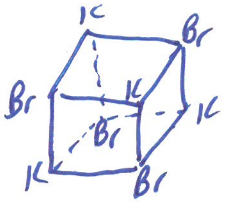
Instructions: Closed book. Put answers in indicated spaces, use notation as given in class & show all work for credit. Insert equation sheet in exam. Answers should have 4-5 significant figures (use more for constants).

1) The crystal structure of potassium bromide (KBr) is simple cubic with the K (ionic effective radius 1.34 Å) and Br (ionic effective radius 1.96 Å) atoms alternating. Find the lattice constant (Å), unit cell volume (m^3), number of K atoms per unit cell, and number Br atoms per unit cell. Then, compute the atomic volume density for the K and Br atoms. Finally, compute the mass density of KBr (g/cm^3).

$$a = 1.34\text{Å} + 1.96\text{Å} = \underline{3.3\text{Å}}$$



$$\text{unit cell vol.} = a^3 = (3.3\times10^{-10})^3$$
$$= \underline{3.5937\times10^{-29}\,m^3}$$



$$\#Br/\text{unit cell} = 4\text{ corners}\left(\frac{1/8\text{ atom}}{\text{corner}}\right) = \underline{0.5}$$
$$\#K/\text{unit cell} = 4\text{ corners}\left(\frac{1/8\text{ atom}}{\text{corner}}\right) = \underline{0.5}$$

$$\text{atomic vol. density}_{K\&Br} = \frac{\#}{a^3} = \frac{0.5}{3.5937\times10^{-29}}$$
$$= \underline{1.391324\times10^{28}\,\text{atoms}/m^3}$$

$$\text{mass density}_{KBr} = \frac{39.098(1.3913\times10^{28}) + 79.904(1.3913\times10^{28})}{6.02214076\times10^{23}}$$
$$= 2.74936\times10^{6}\,g/m^3\ \frac{1\,m^3}{100^3\,cm^3}$$
$$= \underline{2.7494\,g/cm^3}$$

KBr lattice constant = 3.3 Å

unit cell volume = $3.5937\times10^{-29}\,m^3$

\# of K atoms per unit cell = 0.5

\# of Br atoms per unit cell = 0.5

atomic vol. density$_K$ = $1.3913\times10^{28}\,\text{atoms}/m^3$

atomic vol. density$_{Br}$ = $1.3913\times10^{28}\,\text{atoms}/m^3$

mass density$_{KBr}$ = $2.7494\,g/cm^3$

2) An x-ray machine operates at 10^{18} Hz in vacuum. Find the wavelength (Å) and energy (J and eV) of a photon for this x-ray. Energetic electrons colliding with a target material generate the x-ray photons. For electrons initially at rest, calculate the potential difference (V) used to impart the necessary energy to the electrons (assume 100% energy transfer from electron to photon). Determine the velocity (m/s), de Broglie wavelength (Å), and momentum (kg•m/s) of each electron.

$$\lambda = c/f = \frac{2.9979246 \times 10^{8}}{10^{18}} = \underline{2.9979246 \times 10^{-10}\,m}$$

$$E = h\nu = 6.62607015 \times 10^{-34}(10^{18}) = \underline{6.62607 \times 10^{-16}\,J}$$

$$= 6.62607 \times 10^{-16}\,J\left(\frac{1\,eV}{1.602176634 \times 10^{-19}\,J}\right) = \underline{4135.668\,eV}$$

$$\text{Volts} = \frac{E(eV)}{e} = \underline{4135.668\ \text{Volts}}$$

$$KE = E = \tfrac{1}{2} m_0 v_e^2 \Rightarrow v_e = \sqrt{\frac{2E}{m_0}} = \sqrt{\frac{2(6.62607 \times 10^{-16})}{9.1093837 \times 10^{-31}}}$$

$$= \underline{3.814156 \times 10^{7}\,m/s}$$

$$\text{momentum}_e = p_e = m_0 v_e = (9.1093837 \times 10^{-31})(3.814156 \times 10^{7})$$

$$= \underline{3.47446 \times 10^{-23}\,kg\,m/s}$$

$$\lambda_e = \frac{h}{p} = \frac{6.62607 \times 10^{-34}}{3.47446 \times 10^{-23}}$$

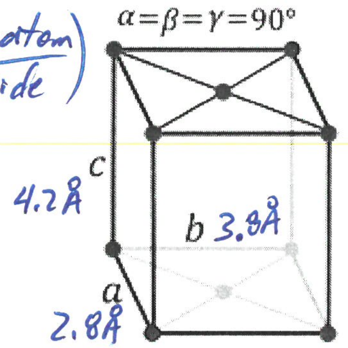
$$= 1.907078 \times 10^{-11}\,m = \underline{0.19071\,Å}$$

$\lambda_{x\text{-ray}}$ = 2.9979 Å   energy$_{x\text{-ray}}$ = 4135.67 eV = 6.62607×10^{-16} J

potential difference$_e$ = 4135.67 V   velocity$_e$ = 3.81416×10^{7} m/s

λ_e = 0.19071 Å   momentum$_e$ = 3.4745×10^{-23} kg m/s

3) A mineral has an end-centered orthorhombic crystal lattice where $a = 2.8$ Å, $b = 3.8$ Å, and $c = 4.2$ Å. Find the number of atoms per unit cell and atomic **volume** density. Then, calculate the number of atoms and atomic **surface** density for the top surface as well as the diagonal surface connecting the back left and front right edges.



$$\frac{\#\text{atoms}}{\text{unit cell}} = 8\text{ corners}\left(\frac{1/8\text{ atom}}{\text{corner}}\right) + 2\text{ sides}\left(\frac{1/2\text{ atom}}{\text{side}}\right)$$

$$= 1+1 = \underline{2}$$

$$\text{atomic vol. density} = \frac{\#\text{atoms}}{abc} = \frac{2}{2.8(3.8)4.2\times10^{-30}}$$

$$= \underline{4.4754744\times10^{28}\ \frac{\text{atoms}}{m^3}}$$

Top Surface $\#\text{atoms}_{top} = 4\text{ corners}\left(\frac{1/4\text{ atom}}{\text{corner}}\right) + 1\text{ side}\left(\frac{1\text{ atom}}{\text{side}}\right)$

$$= 1+1 = 2$$

$$\text{atomic surf. density}_{TOP} = \frac{\#\text{atoms}}{ab} = \frac{2}{2.8(3.8)\times10^{-20}} = 1.879699\times10^{19}\ \frac{\text{atoms}}{m^2}$$

Diagonal Surface $\#\text{atoms}_{BkL-FtR} = 4\text{ corners}\left(\frac{1/4\text{ atom}}{\text{corner}}\right) + 2\text{ sides}\left(\frac{1/2\text{ atom}}{\text{side}}\right)$

$$= 1+1 = \underline{2}$$

$$\text{atomic surf. density}_{BkL-FtR} = \frac{\#\text{atoms}}{\sqrt{a^2+b^2}\,c} = \frac{2}{\sqrt{2.8^2+3.8^2}(10^{-10})4.2\times10^{-10}}$$

$$= \underline{1.0088419\times10^{19}\ \frac{\text{atoms}}{m^2}}$$

atoms/unit cell = 2

atomic volume density = $4.4755\times10^{28}\ \frac{\text{atoms}}{m^3}$

atoms$_{top}$ = 2

atomic surface density$_{top}$ = $1.8797\times10^{19}\ \frac{\text{atoms}}{m^2}$

atoms$_{BkL-FtR}$ = 2

atomic surface density$_{BkL-FtR}$ = $1.0088\times10^{19}\ \frac{\text{atoms}}{m^2}$

4) An electron, located far into $x < 0$, is accelerated from rest by a potential of 0.5 V in the $+x$-direction. At $x = 0$, it encounters a 3 eV potential barrier that is 3.1 Å wide. Find the kinetic energy (eV & J), velocity (m/s), and de Broglie wavelength (Å) of the electron for $x < 0$. Given the potential for $x < 0$ and $x > 3.1$ Å is zero, calculate the wave numbers for $x < 0$ (k_{I}) and $0 < x < 3.1$ Å (k_{II}). Then, determine the exact T_{exact} and approximate T_{aprox} electron tunneling probabilities to $x > 3.1$ Å (unitless and %).

$$KE_e = E = 1\text{electron}(0.5\,V) = \underline{0.5\,eV}$$

$$= (0.5\,eV)\left(1.602176634\times10^{-19}\,\frac{J}{eV}\right) = \underline{8.01088\times10^{-20}\,J}$$

$$KE_e = 0.5\,m v_e^2 \Rightarrow v_e = \sqrt{\frac{2E}{m_0}} = \sqrt{\frac{2(8.01088\times10^{-20})}{9.1093837\times10^{-31}}} = \underline{419{,}382.88\ m/s}$$

$$(2.3)\quad \lambda = \frac{h}{p} = \frac{6.62607015\times10^{-34}}{9.1093837\times10^{-31}(419382.88)} = \underline{1.73443\times10^{-9}}\,m$$

$$(2.61a)\quad k_1 = k_I = \sqrt{\frac{2mE}{\hbar^2}} = \frac{\sqrt{2(9.1093837\times10^{-31})8.01088\times10^{-20}}}{1.05457\times10^{-34}}$$

$$= \underline{3.62263\times10^{9}\ rad/m}$$

$$(2.61b)\quad k_2 = k_{II} = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} = \frac{\sqrt{2(9.1094\times10^{-31})(3-0.5)1.6022\times10^{-19}}}{1.05457\times10^{-34}}$$

$$= \underline{8.10044\times10^{9}\ Np/m}$$

$$k_2 a = 8.10044\times10^{9}(3.1\times10^{-10}) = 2.511136$$

$$T_{exact} = \frac{1}{1+\frac{3^2\sinh^2(2.5111)}{4(0.5)(3-0.5)}} = \underline{0.0146214 = 1.46214\%}$$

$$T_{approx} = 16\,\frac{0.5}{3}\left(1-\frac{0.5}{3}\right)e^{-2(2.51136)} = \underline{0.0146434 = 1.46434\%}$$

$KE_{x<0}$ = $\underline{0.5eV}$ = $\underline{8.0109\times10^{-20}\,J}$ velocity$_{x<0}$ = $\underline{419{,}382.9\ m/s}$

$\lambda_{x<0}$ = $\underline{17.344\ Å}$ k_{I} = $\underline{3.6226\times10^{9}\ rad/m}$ k_{II} = $\underline{8.1004\times10^{9}\ Np/m}$

T_{exact} = $\underline{0.014621}$ = $\underline{1.4621\%}$ T_{aprox} = $\underline{0.014643}$ = $\underline{1.4643\%}$

1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [278]	110 Ds Darmstadtium [281]	111 Rg Roentgenium [280]	112 Cn Copernicium [285]	113 Nh Nihonium [286]	114 Fl Flerovium [289]	115 Mc Moscovium [289]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]

K 39.098 amu

Br 79.904 amu