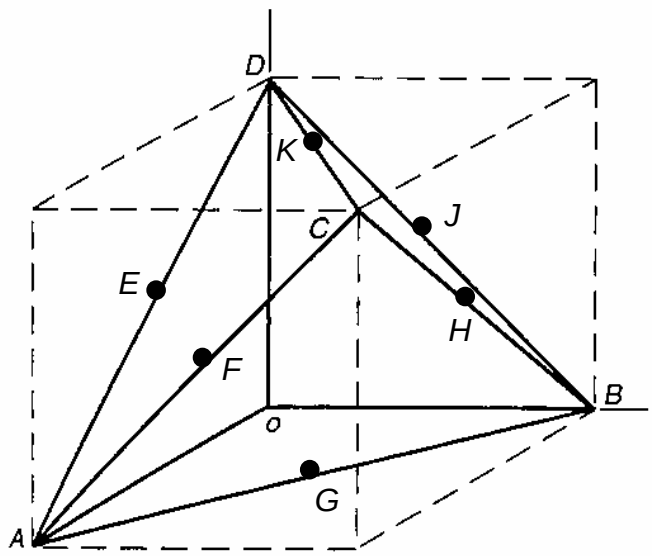
Department of Materials Science and Engineering
Massachusetts Institute of Technology
3.14 Physical Metallurgy – Fall 2003

Solutions to Problem Set #1

1.1 Exercise 1.6. In addition to labeling the faces of the tetrahedron, also indicate the directional indices of the tetrahedron edges and the vectors that lie on the faces and connect the center of an edge to a vertex.



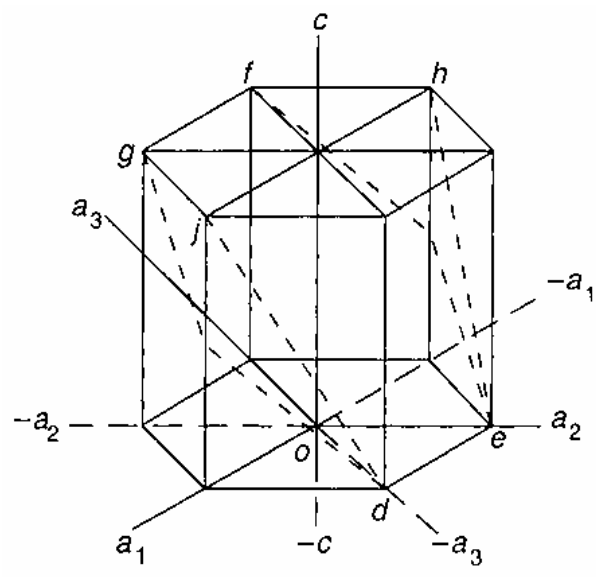
Faces:	ABC	$(11\bar{1})$	Directions in faces:	AK	$[\bar{1}12]$	A	CD
	ABD	(111)		CE	$[\bar{1}\bar{2}\bar{1}]$	C	AD
	ACD	$(1\bar{1}1)$	(in ACD)	DF	$[21\bar{1}]$	D	AC
	BCD	$(\bar{1}11)$		BK	$[1\bar{1}2]$	B	CD
Edges:	AB	$[\bar{1}10]$		CJ	$[\bar{2}\bar{1}\bar{1}]$	C	BD
	AD	$[\bar{1}01]$	(in BCD)	DH	$[12\bar{1}]$	D	BC
	AC	$[011]$		AH	$[\bar{1}21]$	A	BC
	BD	$[0\bar{1}1]$		BF	$[2\bar{1}1]$	B	AC
	BC	$[101]$	(in ABC)	CG	$[\bar{1}\bar{1}\bar{2}]$	C	AB
	CD	$[110]$		AJ	$[\bar{2}11]$	A	BD
				BE	$[1\bar{2}1]$	B	AD
			(in ABD)	DG	$[11\bar{2}]$	D	AB

1.2 Exercise 1.7. In addition, also give the indices of the vectors between points:

i. ***g* and *j***

ii. ***h* and *e***

iii. ***f* and *e***



Direction or plane	Miller indices
(defg)	$(01\bar{1}2)$
(dehj)	$(01\bar{1}1)$
[gj]	$[11\bar{2}0]$
[he]	$[11\bar{2}1]$
[fe]	$[12\bar{3}\bar{1}]$

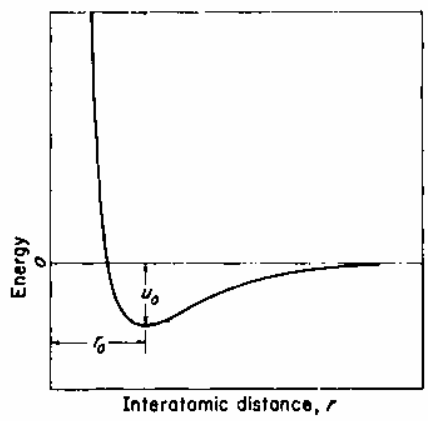
1.3 Draw a pair potential curve for interacting metal species on a graph with axes energy and distance. Using your knowledge of how energies relate to forces and materials properties, describe which features of your potential curve are related to each of the following properties:

i. Tensile strength
ii. Elastic modulus
iii. Melting temperature
iv. Coefficient of thermal expansion

Your pair potential should look roughly like this:

r_o = equilibrium atomic spacing

u_o = cohesive energy



i. The *strength* of the material can be determined from the *depth* of the potential well. Deeper wells (higher cohesive energies) result in higher tensile strengths.

ii. The *elastic modulus* can be determined from the *curvature* of the potential as the modulus is the slope of the force-displacement curve – making it the second derivative of the energy curve.

iii. The *melting temperature* is determined from the *cohesive energy* (or the depth of the potential well). This tells us how much energy we need to add to the system to break the bonds between two atoms. Higher cohesive energies result in higher melting temperatures.

iv. The *coefficient of thermal expansion* is related to the width and asymmetry of the curve near the minimum. At T = 0K, atoms will rest at the minimum energy position (equilibrium lattice spacing). As the temperature increases (add energy to the system), the atoms vibrate between the two sides of the potential curve. If the distance between the equilibrium position and the curve is greater on the right side, the material will seem to expand when heated (material dimension is just an "average" picture of all interatomic spacings). The more the curve is skewed to the right, the higher the thermal expansion will be.

1.4 Exercise 7.10

(a) The vacancy concentration at the melting point can be found from:

$$X_v = \exp\left(-\frac{H_f}{RT_m}\right)$$

Since they give us H_f in eV, we use R = 8.617 x 10^{-5}. T_m must be in K, not degrees C. The final vacancy concentrations are:

Element	H_f (eV)	T_m (ºC)	T_m (K)	X_v
Al	0.76	660	933	7.84E-05
Ag	0.92	961	1234	1.75E-04
Cu	0.9	1083	1356	4.52E-04
Au	0.95	1063	1336	2.61E-04
Ni	1.4	1453	1726	8.17E-05
Pt	1.4	1769	2042	3.50E-04

(b) The results of this problem *do not* support the view that near the melting temperature vacancy concentrations are too high to support a crystal. The concentrations calculated in part (a) correspond to 1 to 5 vacancies per 10,000 atoms. The mean distance between vacancies is ~21.5 atoms, which isn't huge, but still large enough to maintain a crystal structure between vacancies.

1.5 Exercise 7.11

(a) The equilibrium concentration of self-interstitial atoms in Cu is:

$$X_{si} = \exp\left(-\frac{H}{RT}\right) = \exp\left(-\frac{385000\text{J/mol}}{8.3145\text{J/molK}\cdot 1000\text{K}}\right) \approx 7.76 \text{ x } 10^{-21}$$

(b) $$r = A\exp\left(-\frac{H_m + H_f}{RT}\right) = 10^{15}\exp\left(-\frac{9640 + 385000}{8.3145\text{J/molK}\cdot 1000\text{K}}\right) \approx 2.36\times 10^{-6}\text{ /s}$$

Note that this is a very small jump rate, but there is a <u>huge</u> formation enthalpy for these defects, so it makes sense that they don't jump very often. If you didn't include H_f in your equation, you'd have found a jump rate ~10^{14}/s, which is roughly the same frequency as phonon vibrations – and not at all physical!