UNIVERSITY COLLEGE LONDON

EXAMINATION FOR INTERNAL STUDENTS

MODULE CODE	:	**GEOLGG05**
ASSESSMENT PATTERN	:	**GEOLGG05A**
MODULE NAME	:	**Earth and Planetary Materials**
DATE	:	**12 May 2016**
TIME	:	**10:00 am**
TIME ALLOWED	:	**2 hours 30 mins**

This paper is suitable for candidates who attended classes for this module in the following academic year(s):

2015/16

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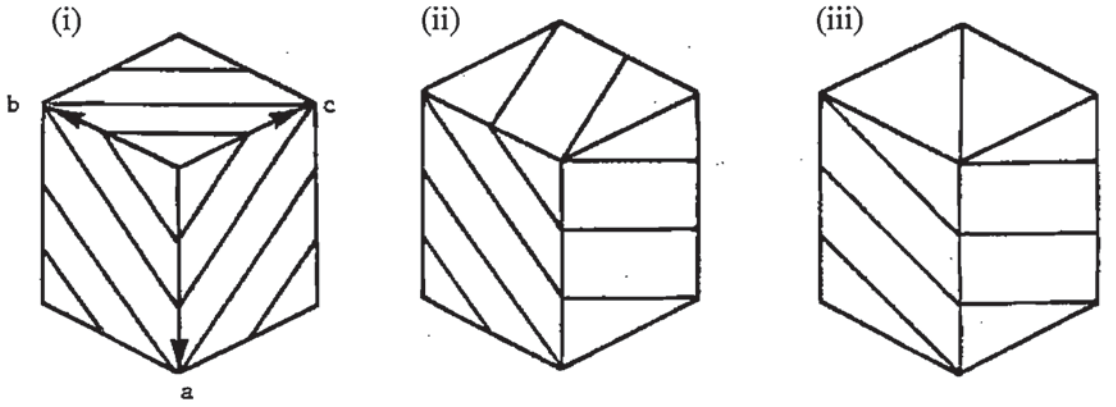
GEOLM006_GG05 EARTH & PLANETARY MATERIALS

*Answer **THREE** questions. All questions carry equal marks. Where a question consists of more than one part (a, b, c etc.) all parts carry equal weight unless stated otherwise. Please hand in Supplement 1 with your answer booklet. You may use a standard electronic calculator. You will be provided with graph paper and tracing paper.*

1. (a) Using the axes as shown on the left in (i) throughout, determine the Miller indices of the 3 sets of planes shown in the diagrams below. [12%]



(b) How does a Primitive (*P*) unit cell differ from a body-centred (*I*) unit cell? What pair of fractional coordinates is produced by body-centring? [10%]

(c) The accompanying supplementary sheet (Supplement 1) shows an incomplete diagram for space group *Pba*2. The diagram is drawn in the conventional orientation, with the *a*-axis running down the page, the *b*-axis running across the page and the *c*-axis coming out of the plane of the paper.

(i) Mark the symmetry elements of *Pba*2 in the blank diagram to the right of the diagram showing the equivalent positions. [16%]

(ii) By inspection of the diagram, list the fractional coordinates of the 4 general equivalent positions. [12%]

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(d) The mineral pyrite crystallizes in the cubic space group *Pa*3, with cell parameter a = 5.41 Å. The Fe atoms occupy the 4a sites with fractional coordinates 0, 0, 0 and the sulfur atoms occupy the 8c sites with fractional coordinates 0.386, 0.386, 0.386.
(i) Calculate the density of pyrite
(Relative atomic masses of Fe and S are 55.85 and 32.06, respectively; Avogadro's number = 6.022×10^{23}) [10%]

With the aid of the space group table (Supplement 2) and graph paper provided:
(ii) Write down the fractional coordinates of all of the atoms in the unit cell [12%]

(iii) Sketch a projection of the crystal structure viewed along [001], indicating on your diagram the relative "heights" of the atoms. [18%]

(iv) Calculate the length of the Fe-S bond. [10%]

2. (a) Describe the use of neutron diffraction in mineralogy. In your answer you should discuss: (i) the advantages and disadvantages of neutron diffraction, when compared to X-ray diffraction, for mineralogical studies, (ii) the methods used for the production of neutrons, (iii) the diffraction geometry and sample environments commonly employed, (iv) the use of Rietveld refinement in the interpretation of neutron powder diffraction patterns, and (v) some recent applications of the technique to Earth & Planetary sciences.

[70%]

(b) For structures with a centre of symmetry, the structure factor for X-ray diffraction is given by

$$F(hkl) = \sum_{n=1}^{N} f_n \cos\left[2\pi\left(hx_n + ky_n + lz_n\right)\right]$$

where the summation is taken over all of the atoms in the unit cell.

The mineral sylvite (KCl) crystallizes with an F-centred cubic unit cell containing four formula units. The atoms occupy the following sites:

K+ ions at:	0, 0, 0	½, ½, 0	0, ½, ½	½, 0, ½
Cl- ions at:	½, 0, 0	0, ½, 0	0, 0, ½	½, ½, ½.

(i) Using the formula above, or otherwise, calculate the structure factors for the 111 and 200 Bragg reflections in terms of the scattering factors of the K^+ and Cl^- ions. [20%]

(ii) The Bragg reflections from this compound can be divided into two categories, weak reflections and strong reflections. Given that the atomic numbers of K and Cl are 19 and 17 respectively, assign the 111 and 200 reflections to these categories. [5%]

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(iii) For neutron diffraction, the structure factor is calculated in exactly the same way, except that the atomic scattering factor, f_n, is replaced by the neutron scattering length, b_n. The values of b for K and Cl are 3.67 fm and 9.58 fm respectively. How will the relative strength of the 111 and 200 reflections in the neutron diffraction pattern differ from that in the X-ray diffraction pattern?

[5%]

3. (a) At moderately high pressure and temperature, NiSi crystallises in the orthorhombic crystal system with space group *Pmmn*.
The *n*-glide in this space group lies perpendicular to the *c*-axis of the unit cell, and the fractional coordinates of those atoms related by this glide are, therefore, given by x, y, z and $\frac{1}{2} + x, \frac{1}{2} + y, -z$.
This space group has a centre of symmetry and the structure factor for X-ray diffraction may be written as

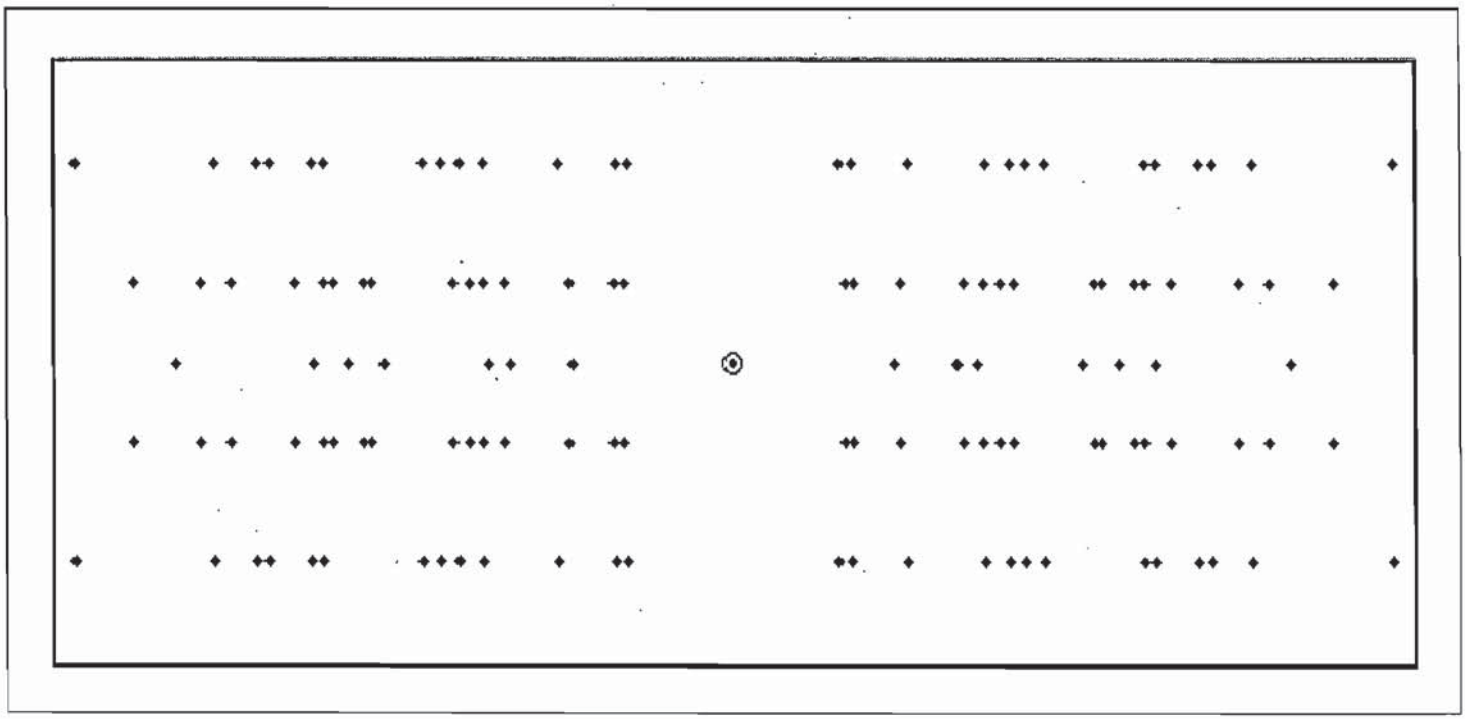
$$F(hkl) = \sum_{n=1}^{N} f_n \cos\left[2\pi\left(hx_n + ky_n + lz_n\right)\right]$$

where the symbols have their usual meanings.

By writing the structure factor as a sum over the pairs of atoms, show that $h\ k\ 0$ Bragg reflections will only be observed from this crystal if $h+k$ is an even number.

[30%]

(b) The diagram below shows a simulated rotation photograph of this form of NiSi, taken using Cu Kα radiation ($\lambda = 1.542$ Å) and a cylindrical camera of radius 30mm. The rotation axis is [001] (i.e. the *c*-axis), and the centre of the diffraction pattern is marked with a small dot surrounded by a circle. By measuring the layer-line spacing, determine the length of the *c*-axis of NiSi. [20%]



TURN OVER

(c) Measure the 2θ values of the seven diffraction spots on the zero layer, which will all have indices *hk0*.
The lengths of the other two axes of the unit cell of NiSi are $a = 3.274$ Å and $b = 3.027$ Å; draw the *hk0* section of the reciprocal lattice (you need only consider the quadrant for which both h and k are ≥ 0) and find the indices of these seven diffraction spots by means of the Ewald circle construction. [50%]

Note: You should include your diagrams of the reciprocal lattice and of the Ewald circle with your answer. Suggested scaling for drawing the reciprocal lattice is $d^* = \lambda / d$ *(i.e.* $C = \lambda$*) and 10 cm = 1 reciprocal lattice unit.*

4. (a) Describe how *diamond-anvil cells* (DACs) may be used to study the structures of minerals at high pressure. In your answer you should explain, with diagrams where appropriate, the operation of the cell, the methods used to ensure that the sample is subject to hydrostatic pressure, and the way in which the pressure on the sample may be determined. [30%]

(b) DACs are often used in combination with *Synchrotron Radiation*. How is this form of radiation generated and why is it especially suitable for use with DACs? [10%]

(c) What are the *perovskite* and *post-perovskite* structures and why are they important in understanding the Earth's lower mantle? In your answer you should include discussion of: (i) the ways in which the perovskite structure can distort from its ideal cubic form, (ii) the ways in which X-ray and neutron diffraction may be used to determine the structural distortions in perovskites, (iii) the perovskite to post-perovskite transition and (iv) the possible structures that may be derived from the post-perovskite structure at higher pressures [60%]

5. (a) Describe how you might use X-ray diffraction to identify the minerals present in a powdered sample of a rock that is thought to contain more than one mineral. Include in your description details of: (i) the method you would use to produce the X-ray beam, (ii) the method you would use to record the diffraction pattern and (iii) the method you would use to interpret the data and identify the minerals present. You should also discuss the possible pitfalls and difficulties that you might encounter when using this method. [50%]

(b) Majorite, $Mg_3(Al,Mg,Si)_2Si_3O_{12}$, is a cubic mineral. The first six Bragg reflections in its powder diffraction pattern (recorded with a wavelength of 1.5406 Å) occur at 2θ values of 18.94°, 21.91°, 29.12°, 31.17°, 34.97°, 36.73°

(i) Calculate the d-spacings of these six reflections [12%]

CONTINUED

(ii) The *d*-spacing of the *hkl* reflection from a cubic crystal is given by the expression

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

The cell parameter of majorite, *a*, is approximately 11.5 Å. Using this value of *a*, and the values of *d* (from (i) above), determine the indices of these six Bragg reflections. [18%]

(iii) Is the unit cell of majorite primitive (*P*), body-centred (*I*) or face-centred (*F*)? [10%]

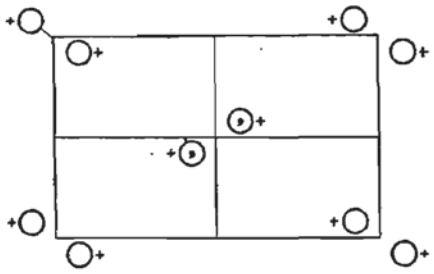
(iii) Using the reflection with the highest Bragg angle, calculate the value of *a* to five significant figures. [10%]

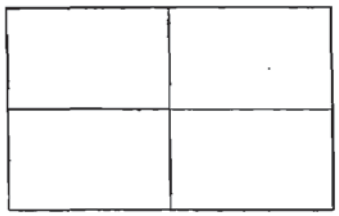
END OF PAPER

Supplement 1 for Question 1c **Candidate Number** .....

$Pba2$
C_{2v}^{8}

No. 32 $P\,b\,a\,2$ $m\,m\,2$ Orthorhombic





Origin on 2

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	c	1		hkl: No conditions $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: No conditions $h00$: $(h=2n)$ $0k0$: $(k=2n)$ $00l$: No conditions
				Special: as above, plus
2	b	2	$0,\frac{1}{2},z$; $\frac{1}{2},0,z$.	hkl: $h+k=2n$
2	a	2	$0,0,z$; $\frac{1}{2},\frac{1}{2},z$.	

Symmetry of special projections

(001) pgg; $a'=a$, $b'=b$ (100) $pm1$; $b'=b/2$, $c'=c$ (010) $p1m$; $c'=c$, $a'=a/2$

END OF SUPPLEMENT 1

GEOLGG05 Handout 1

Supplement 2 for Question 1d

$Pa3$ T_h^6

No. 205 $P\,2_1/a\,\bar{3}$ $m\,3$ Cubic

Origin at centre ($\bar{3}$)

24	*d*	1	x,y,z; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; z,x,y; $\frac{1}{2}+z,\frac{1}{2}-x,\bar{y}$; $\bar{z},\frac{1}{2}+x,\frac{1}{2}-y$; $\frac{1}{2}-z,\bar{x},\frac{1}{2}+y$; y,z,x; $\frac{1}{2}+y,\frac{1}{2}-z,\bar{x}$; $\bar{y},\frac{1}{2}+z,\frac{1}{2}-x$; $\frac{1}{2}-y,\bar{z},\frac{1}{2}+x$; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$; $\frac{1}{2}+x,y,\frac{1}{2}-z$; $\bar{z},\bar{x},\bar{y}$; $\frac{1}{2}-z,\frac{1}{2}+x,y$; $z,\frac{1}{2}-x,\frac{1}{2}+y$; $\frac{1}{2}+z,x,\frac{1}{2}-y$; $\bar{y},\bar{z},\bar{x}$; $\frac{1}{2}-y,\frac{1}{2}+z,x$; $y,\frac{1}{2}-z,\frac{1}{2}+x$; $\frac{1}{2}+y,z,\frac{1}{2}-x$.	General: *hkl*: No conditions 0*kl*: $k=2n$ *h*0*l*: $(l=2n)$ *hk*0: $(h=2n)$ *h*, *k*, *l* not permutable
8	*c*	3	x,x,x; $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x}$; $\bar{x},\frac{1}{2}+x,\frac{1}{2}-x$; $\frac{1}{2}-x,\bar{x},\frac{1}{2}+x$; $\bar{x},\bar{x},\bar{x}$; $\frac{1}{2}-x,\frac{1}{2}+x,x$; $x,\frac{1}{2}-x,\frac{1}{2}+x$; $\frac{1}{2}+x,x,\frac{1}{2}-x$.	Special: as above, plus no extra conditions
4	*b*	$\bar{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$.	} *hkl*: $h+k,k+l,(l+h)=2n$
4	*a*	$\bar{3}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$; $\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.	

END OF SUPPLEMENT 2

GEOLGG05 Handout 2