

2017

Integrated Graduate School of Medicine, Engineering, and Agricultural Sciences, Doctoral Course, University of Yamanashi

Entrance Examination

No. 1/3

Course or Program	Special Doctoral Program for Green Energy Conversion Science and Technology	Subject	Solid State Physics
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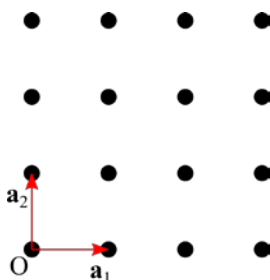
Question 1

(1) Write Bragg's equation and explain the equation with illustration.

(2) Relationship between fundamental vectors of real lattice ( $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ ) and reciprocal lattice ( $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ ) can be expressed by following formula.

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_2 \times \mathbf{a}_3 \cdot \mathbf{a}_1}, \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_3 \times \mathbf{a}_1 \cdot \mathbf{a}_2}, \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \times \mathbf{a}_2 \cdot \mathbf{a}_3}$$

Figure below shows projected real primitive lattice in the direction of  $\mathbf{a}_3$ . Please duplicate the real lattice into your answer sheet, and draw reciprocal lattice and 1st Brillouin zone. (The reciprocal lattice may have an arbitrary size.)



Question 2

Following table shows some properties of each crystal composed of elemental substance in period-four transition metals and typical elements. From this table, densities of Ga and Ge are apparently smaller than those of Fe, Co, Ni, Cu and Zn. Answer the reason for such small density in terms of bond species and crystal structure.

element	Fe	Co	Ni	Cu	Zn	Ga	Ge
atomic weight / $\text{g} \cdot \text{mol}^{-1}$	55.85	58.93	58.69	63.55	65.39	69.72	72.61
density of crystal / $\text{g} \cdot \text{cm}^{-3}$	7.87	8.90	8.91	8.93	7.13	5.91	5.32
minimum interatomic distance / $\text{\AA}$	2.48	2.50	2.49	2.56	2.66	2.44	2.45

<bond species>

<crystal structure>

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Question 3

Let us consider an eclipsed stack of virtual square planar  $d^8$  NiH<sub>4</sub> complexes along with  $z$ -axis (Fig.3-1).

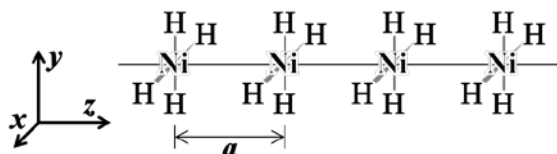


Fig.3-1.

Ignoring the mixing between Ni and H ligands and secondary mixing; eg. mixing between Ni  $4p_z$  and Ni  $3d_{z^2}$  in the polymer. Only a band which is formed by each independent molecular orbital is considered: For example, do not take account of a band formed by  $p_z$  and  $d_{z^2}$ .

- (1) Which types of molecular orbitals are formed: (a)  $4p_z$ , (b)  $3d_{xy}$ , (c)  $3d_{xz}$ , (d)  $3d_{yz}$ , (e)  $3d_{z^2}$ , and (f)  $3d_{x^2-y^2}$ .
- (2) The schematic energy diagram of the orbitals listed in Q(1) is shown in Fig.3-2. Draw the schematic band structure which is assumed by band width and orbital topology using an example from  $E(k)$  curve of a chain of H  $1s$  orbitals with a separation of  $a$  (Fig.3-3).
- (3) Draw a schematic density of states (DOS) curves of the band structure drawn in Q(2).

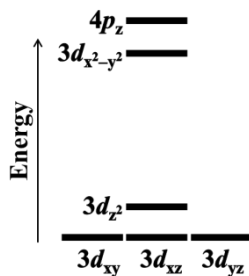


Fig.3-2.

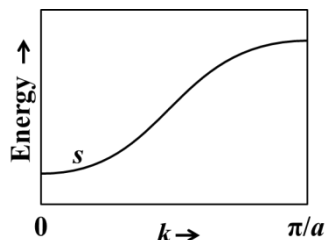


Fig.3-3.

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Question 4

- (1) Answer the electronic configurations of  $\text{Cr}^{3+}$ ,  $\text{Fe}^{3+}$ , and  $\text{Gd}^{3+}$ . (Atomic numbers of Cr, Fe, and Gd are 24, 26, and 64, respectively.)
- (2) Fig.4-1 shows the Brillouin function of the compounds of  $\text{Cr}^{3+}$ ,  $\text{Fe}^{3+}$ , and  $\text{Gd}^{3+}$ . Specify the compounds which belong to each of the curve (a), (b), and (c).
- (3) Under low magnetic field and high temperature, the Brillouin function can be approximated by a law. Answer the law name and the equation.

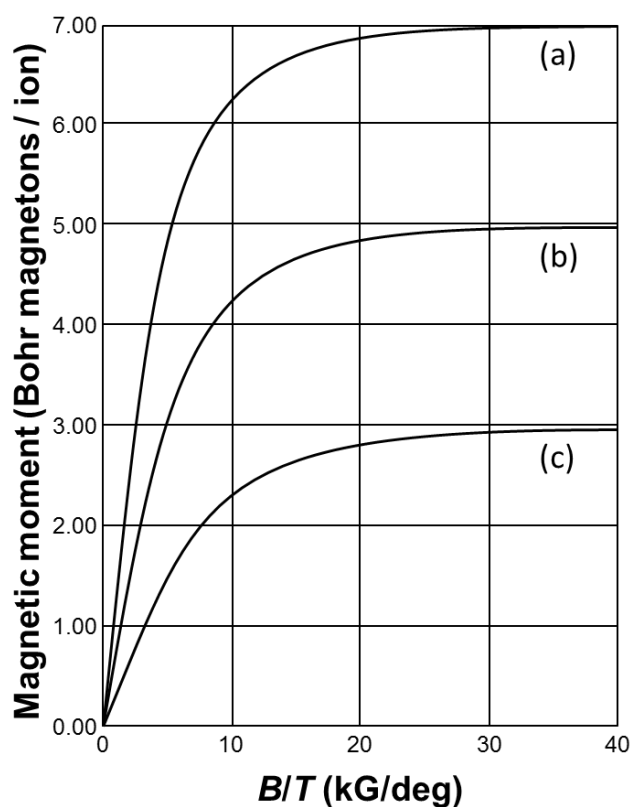


Fig.4-1.