ΕΕΝ, τελικό 2009

① $\lambda = \frac{A}{M} = \frac{A}{\rho V}$ (α) $\lambda = \frac{4\pi (d/2)^2}{\frac{4}{3}\pi (\frac{d}{2})^3 \rho} = \frac{6}{d\rho} \rightarrow \lambda = 1.0\ cm^2/g$

(β) $\lambda = \frac{A}{\rho A d} = \frac{1}{d\rho} \rightarrow \lambda = 4.0\ cm^2/g$ (γ) $\lambda = \frac{6a^2}{a^3\rho} = \frac{6}{a\rho} \rightarrow \lambda = 4.8\cdot 10^5 \frac{cm^2}{g}$

(δ) κόστος $\kappa = 180 \frac{€}{g} m = 180 \frac{€}{g} \frac{A}{\lambda} = 180 \frac{€}{g} \frac{0.1 \cdot 10^4 cm^2}{\lambda}$

$\rightarrow \kappa = 1.8\cdot 10^5 / (\lambda / cm^2/g)$ € άρα (α) → 180000€, (β) → 45000€, (γ) → 0.38€.

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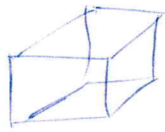
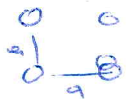
② (α) $E_{db} = \frac{E_c}{6} = \frac{200\cdot 10^3\ J/mol}{6\cdot 6\cdot 10^{23}\ mol^{-1}} = 5.6\cdot 10^{-20}\ J$



(α)

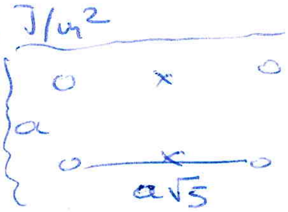


$\gamma_{100} = \frac{1\cdot E_{db}}{a^2} = E_{db}/a^2 \rightarrow \gamma_{100} = 0.51\ J/m^2$

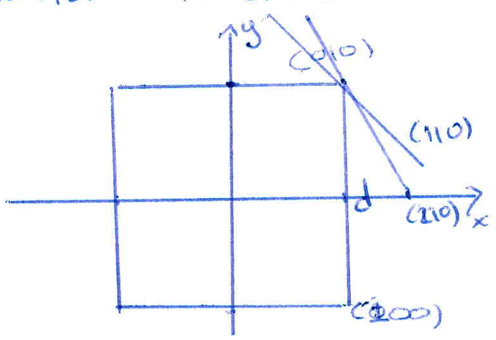
$\gamma_{110} = \frac{2\cdot E_{db}}{a a\sqrt{2}} = \sqrt{2}\frac{E_{db}}{a^2} = \sqrt{2}\gamma_{100} \rightarrow \gamma_{110} = 0.72\ J/m^2$

$\gamma_{111} = \frac{3 E_{db}}{(a\sqrt{2})^2 \sqrt{3}/2} = \sqrt{3}\frac{E_{db}}{a^2} = \sqrt{3}\gamma_{100} \rightarrow \gamma_{111} = 0.88\ J/m^2$

$\gamma_{210} = \frac{3E_{db}}{a a\sqrt{5}} = \frac{3\sqrt{5}}{5}\frac{E_{db}}{a^2} = \frac{3\sqrt{5}}{5}\gamma_{100} \rightarrow \gamma_{210} = 0.68\ J/m^2$



Το σχήμα θα είναι κύβος, με ίσως κομμένες ακμές και γωνίες. Στο επίπεδο (100) που περνά από το κέντρο:



$d_{100} = d$ $d_{110} = \frac{\gamma_{110}}{\gamma_{100}} d = \sqrt{2} d$ άρα το (110) οριακά δεν εμφανίζεται

$d_{210} = \frac{3\sqrt{5}}{5} d$ έστω εξίσωση $2x+y=c$

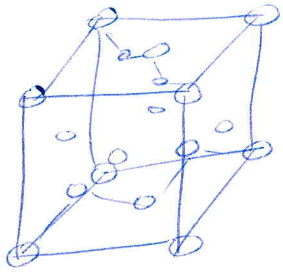
$d_{210} = \frac{c}{\sqrt{2^2+1^2}} = \frac{c}{\sqrt{5}} = \frac{3\sqrt{5}}{5} d \rightarrow c = 3d$

άρα $y = 3d-2x > d$ για $-d<x<d$

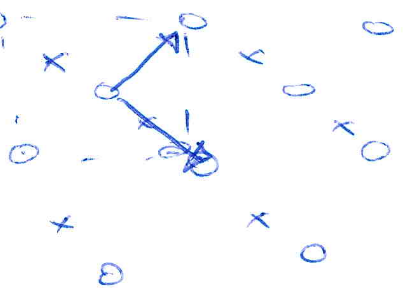
και $x = (3d-y)/2 > d$ για $y<d$ άρα κι αυτό πέφτει εκτός του τετραγώνου

Το (111) θα έχει $d_{111} = \sqrt{3} d$ άρα εξίσωση $x+y+z = 3d$ άρα αφού στον κύβο $-d<y<d$, $-d<z<d \Rightarrow x>d$ ή $x<-d$ άρα κι αυτό πέφτει εκτός. Άρα μόνο η (100) θα εμφανιστεί στο σχήμα ελάχιστης ενέργειας το οποίο θα είναι κύβος.

(3)



(α) o = επιφάνεια
x = 2ο επίπεδο



δεσμός $d = \left|\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)\right| = a\frac{\sqrt{3}}{4} \rightarrow 2R = \frac{a\sqrt{3}}{4}$

$\Rightarrow R = a\sqrt{3}/8$

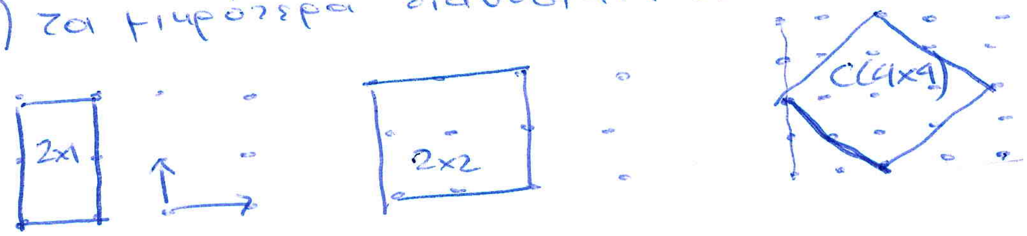
$$f = \frac{\pi R^2}{a^2/2} = \frac{\pi a^2 3}{64 a^2/2} = \frac{3\pi}{32} \rightarrow \boxed{f = 0.29}$$

$$\boxed{n_s = \frac{2}{a^2}} \qquad \gamma = \frac{(2+2)E_{db}}{a^2} = \frac{4E_{db}}{a^2} = \frac{4(E_c/4)}{a^2} \rightarrow \boxed{\gamma = \frac{E_c}{a^2}}$$

(β) $R \approx 2Å \rightarrow a = \frac{8}{\sqrt{3}}R \approx 5Å \rightarrow n_s = \frac{2}{a^2} \approx 0.1 Å^{-2} = \underline{10^{15} cm^{-2}}$

$E_{db} \sim eV \rightarrow E_c \sim 5 eV \rightarrow \gamma = \frac{1}{5} eV/Å^2 = \frac{1.6\cdot 10^{-19} J}{5\cdot 10^{-20} m^2} \sim \underline{1 J/m^2}$

(γ) τα μικρότερα διανύσματα είναι αυτά του σχήματος



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(4) $H_2 + 2* \underset{k_H^d}{\overset{k_H^a}{\rightleftharpoons}} 2H*$ $\qquad \theta_H = \sqrt{K_H P_{H_2}}\,\theta_*$ (1)

$CO + * \underset{k_{CO}^d}{\overset{k_{CO}^a}{\rightleftharpoons}} CO*$ $\qquad \theta_{CO} = K_{CO}P_{CO}\,\theta_*$ (2)

$\theta_H + \theta_{CO} + \theta_* = 1 \Rightarrow \theta_* = 1/\left(1 + K_{CO}P_{CO} + \sqrt{K_H P_{H_2}}\right)$ (3)

αντικαθιστώ την (3) στις (1), (2) και τελειώσαμε

$P_{H_2} + P_{CO} = P \rightarrow P_{H_2} \approx P = 1 bar = 10^5 Pa$

$P_{CO} \approx x P$.

άρα στους τύπους $p_{H_2} = P_{H_2}/P \approx 1$, $\quad p_{CO} = \frac{P_{CO}}{P} \approx x$

$$K_H = \frac{k_H^a}{k_H^d} = \frac{Z_H A_{at}}{\nu e^{-E_d^H/RT}}, \quad K_{CO} = \frac{k_{CO}^a}{k_{CO}^d} = \frac{Z_{CO}A_{at}}{\nu e^{-E_d^{CO}/RT}}$$

$$A_{at} = \left(\frac{1}{\left(\frac{a\sqrt{2}}{2}\right)^2\frac{\sqrt{3}}{2}}\right)^{-1} = \left(\frac{4}{\sqrt{3}a^2}\right)^{-1} = \frac{\sqrt{3}}{4}a^2 = 6.7\cdot 10^{-20} m^2$$

$$Z_H = \frac{P}{\sqrt{2\pi m_{H_2} k_B T}}, \quad Z_{CO} = \frac{P}{\sqrt{2\pi m_{CO} k_B T}} \rightarrow \begin{array}{l} K_H = 1.3\cdot 10^8 \\ K_{CO} = 1.1\cdot 10^{10} \end{array}$$

x	θ_{CO}	θ_H	θ_*
10^{-6}	0.49	0.51	0
10^{-5}	0.91	0.09	0
10^{-4}	0.99	0.01	0