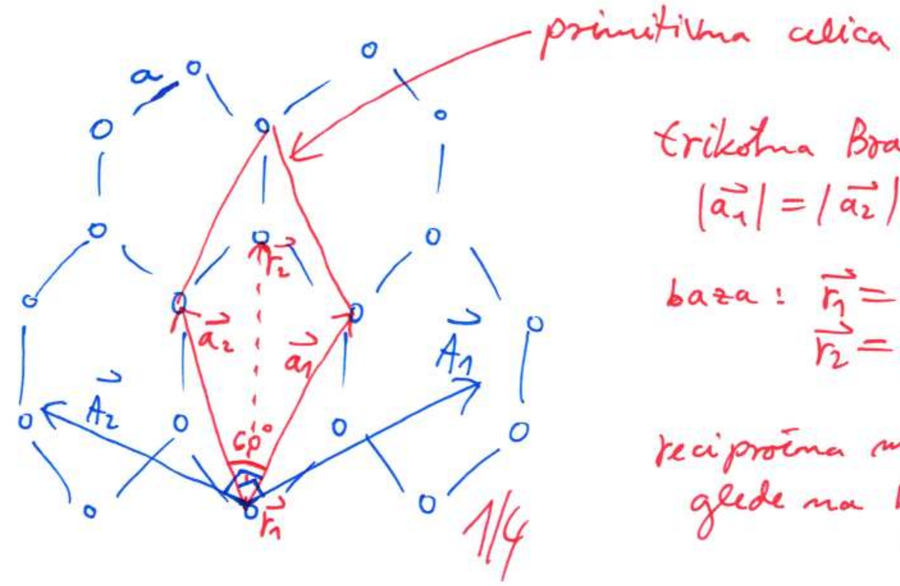
① a)



trikotna Bravaisova mreža

$|\vec a_1| = |\vec a_2|$, $\sphericalangle \vec a_1, \vec a_2 = 60°$

baza: $\vec r_1 = 0$

$\vec r_2 = \frac{2}{3}(\vec a_1 + \vec a_2)$

recipročna mreža: trikotna, glede na BM zasukana za 30° (vaje)

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b) $S_{\vec K} = e^{i\vec K\cdot\vec r_1} + e^{i\vec K\cdot\vec r_2} = 1 + e^{i(m_1\vec A_1 + m_2\vec A_2)\cdot\frac{2}{3}(\vec a_1+\vec a_2)} =$

$= 1 + e^{i\frac{4\pi}{3}(m_1+m_2)}$

$$S_{\vec K} = \begin{cases} 2\ ; & m_1+m_2 = 3n \\ 1+e^{i\frac{4\pi}{3}}\ ; & m_1+m_2 = 3n+1 \\ 1+e^{-i\frac{4\pi}{3}}\ ; & m_1+m_2 = 3n-1 \end{cases} \qquad (n\in\mathbb{Z})$$

$S_{\vec K}$ je različen od 0 za vsako kombinacijo Millerjevih indeksov m_1 in m_2.

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c) $2d\sin\frac{\vartheta}{2} = \lambda$; $d = \frac{2\pi}{|\vec K|}$; $|\vec K| = |m_1\vec A_1 + m_2\vec A_2| =$

$= \sqrt{m_1^2|\vec A_1|^2 + m_2^2|\vec A_2|^2 + 2m_1m_2|\vec A_1||\vec A_2|\cos(120°)} =$

$= \frac{4\pi}{3a}\sqrt{m_1^2+m_2^2-m_1m_2}$

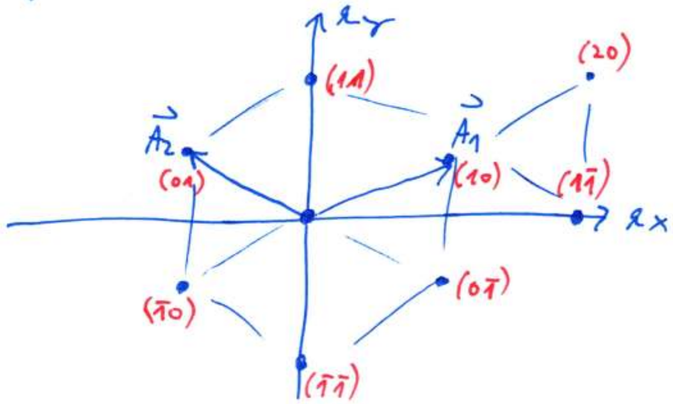
$$\left(\begin{aligned} &\vec a_1\cdot\vec A_1 = |\vec a_1||\vec A_1|\cdot\cos 30° = 2\pi \\ &|\vec A_1| = |\vec A_2| = \frac{2\pi}{|\vec a_1|\cos 30°} = \frac{4\pi}{3a} \\ &|\vec a_1| = \sqrt{\left(\tfrac{3}{2}a\right)^2 + \left(\tfrac{\sqrt3}{2}a\right)^2} = \sqrt3 a \end{aligned}\right)$$

$d = \frac{3a}{2\sqrt{m_1^2+m_2^2-m_1m_2}}$

$\sin\frac{\vartheta}{2} = \frac{\lambda}{2d} = \frac{\lambda}{3a}\sqrt{m_1^2+m_2^2-m_1m_2}$

$\frac{\lambda}{3a} = 0.437 \Rightarrow m_1^2+m_2^2-m_1m_2 \leq 5$

recipročna mreža:



$\{10\} \rightarrow \vartheta = 51.8°$

$\{1\bar1\} \rightarrow \vartheta = 98.3°$

$\{20\} \rightarrow \vartheta = 121.7°$

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① d) "AA stacking": Bravaisova mreža, primitivna celica in recipročna mreža ostanejo take, kot pri grafenu.

$$\text{baza:} \quad \vec{r_1} = \vec{r_3} = 0$$
$$\vec{r_2} = \vec{r_4} = \frac{2}{3}(\vec{a_1} + \vec{a_2})$$

$$S_{\vec{k}} = 2 S_{\vec{k}}^{grafen}$$

$$\text{intenziteta:} \quad I_{\vec{k}} \propto \left|\frac{N}{2} S_{\vec{k}}\right|^2 = \left|N S_{\vec{k}}^{grafen}\right|^2$$

(N: število primitivnih celic kristala grafena
$\frac{N}{2}$: število primitivnih celic kristala dvoplastnega grafena)

Uklonski vrhovi se pojavijo pri enakih uklonskih kotih, kot pri grafenu, tudi njihove intenzitete se ne spremenijo.

"AB stacking": Bravaisova mreža, primitivna celica in recipročna mreža ostanejo take, kot pri grafenu.

$$\text{baza:} \quad \vec{r_1} = 0$$
$$\vec{r_2} = \frac{2}{3}(\vec{a_1} + \vec{a_2})$$
$$\vec{r_3} = \frac{1}{3}(\vec{a_1} + \vec{a_2})$$
$$\vec{r_4} = \frac{2}{3}(\vec{a_1} + \vec{a_2})$$

$$S_{\vec{k}} = 1 + e^{i\frac{2\pi}{3}(m_1+m_2)} + 2e^{i\frac{4\pi}{3}(m_1+m_2)}$$

$$S_{\{10\}} = 1 + e^{i\frac{2\pi}{3}} + 2e^{i\frac{4\pi}{3}} = e^{i\frac{4\pi}{3}} \qquad S_{\{10\}}^{grafen} = -e^{-i\frac{2\pi}{3}}$$

$$S_{\{1\bar{1}\}} = 1 + 1 + 2 = 4 \qquad S_{\{1\bar{1}\}}^{grafen} = 2$$

$$S_{\{20\}} = 1 + e^{i\frac{4\pi}{3}} + 2e^{i\frac{8\pi}{3}} = e^{i\frac{2\pi}{3}} \qquad S_{\{20\}}^{grafen} = -e^{i\frac{4\pi}{3}}$$

$$I_{\{10\}} \propto \left|\frac{N}{2} S_{\{10\}}\right|^2 \Rightarrow \quad I_{\{10\}} = \frac{1}{4} I_{\{10\}}^{grafen}$$

$$I_{\{1\bar{1}\}} \propto \left|\frac{N}{2} S_{\{1\bar{1}\}}\right|^2 \Rightarrow \quad I_{\{1\bar{1}\}} = I_{\{1\bar{1}\}}^{grafen}$$

$$I_{\{20\}} \propto \left|\frac{N}{2} S_{\{20\}}\right|^2 \Rightarrow \quad I_{\{20\}} = \frac{1}{4} I_{\{20\}}^{grafen}$$

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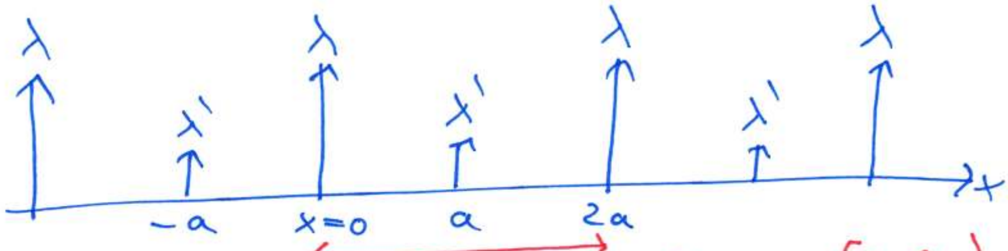
Uklonski vrhovi pri enakih kotih, kot pri grafenu. Intenziteta vrha pri 98.3° ostane enaka, medtem ko se intenzitete vrhov pri 51.8° in 121.7° zmanjšajo za faktor 4.

② a)



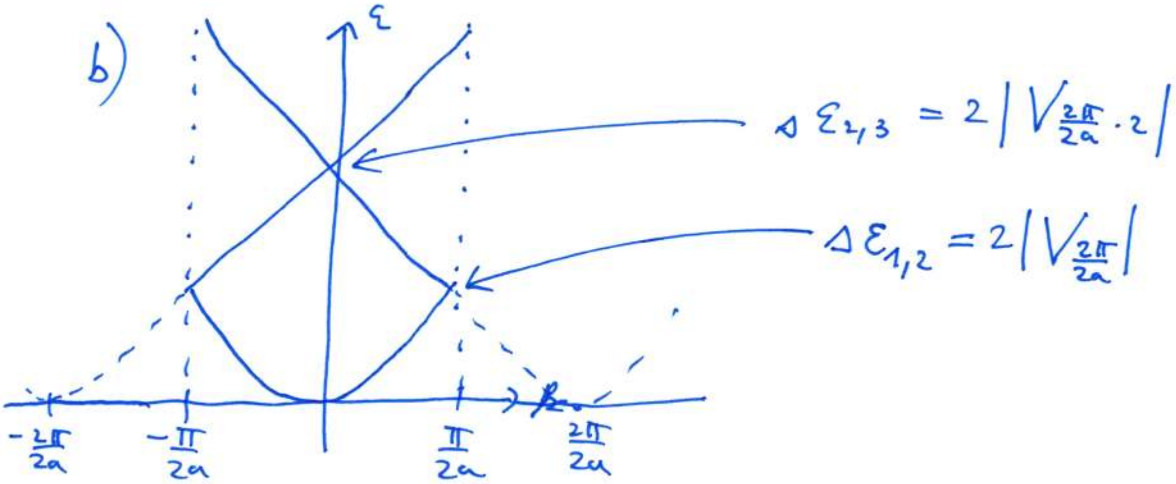
primitivna celica: $[0, 2a)$

baza: $x_1 = 0$
$x_2 = a$

recipročna mreža: $\frac{2\pi}{2a} m$; $m \in \mathbb{Z}$

1. Brillouinova cona: $\left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right)$ 1/4 +

b)



$$V_{\frac{2\pi}{2a}\cdot m} = \frac{1}{2a}\int_{0_-}^{(2a)_-} V(x) e^{-i\frac{2\pi}{2a}m x} dx = \frac{1}{2a}\left(\lambda + \lambda' e^{-im\pi}\right)$$

$$\Delta \varepsilon_{1,2} = \frac{\lambda - \lambda'}{a}, \quad \Delta \varepsilon_{2,3} = \frac{\lambda + \lambda'}{a} \longrightarrow \lambda = \frac{(\Delta \varepsilon_{1,2} + \Delta \varepsilon_{2,3})\, a}{2} = \underline{\underline{0.32\,\text{eVnm}}}$$

$$\lambda' = \frac{(\Delta \varepsilon_{2,3} - \Delta \varepsilon_{1,2})\, a}{2} = \underline{\underline{0.08\,\text{eVnm}}}$$

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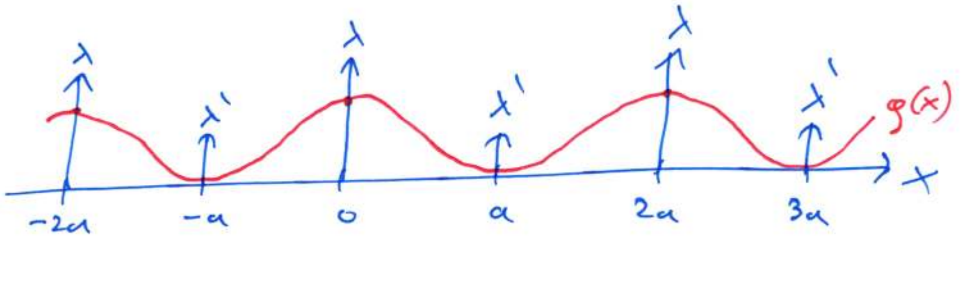
c)
$$\begin{bmatrix} -\left|V_{\frac{2\pi}{2a}}\right|, & V_{\frac{2\pi}{2a}} \end{bmatrix} \begin{bmatrix} C_{\frac{\pi}{2a}-0} \\ C_{\frac{\pi}{2a}-\frac{2\pi}{2a}} \end{bmatrix} = 0 \Rightarrow \begin{bmatrix} C_{\frac{\pi}{2a}-0} \\ C_{\frac{\pi}{2a}-\frac{2\pi}{2a}} \end{bmatrix} \propto \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\psi(x) \propto 1 \cdot e^{i\left(\frac{\pi}{2a}-0\right)x} + 1 e^{i\left(\frac{\pi}{2a}-\frac{2\pi}{2a}\right)x} \propto \cos\frac{\pi x}{2a}$$

$$\rho(x) = |\psi(x)|^2 \propto \cos^2\frac{\pi x}{2a}$$



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