X-ray Photoelectron Spectroscopy as a tool for control superlattice heterostructures quality and surface bilayer formation

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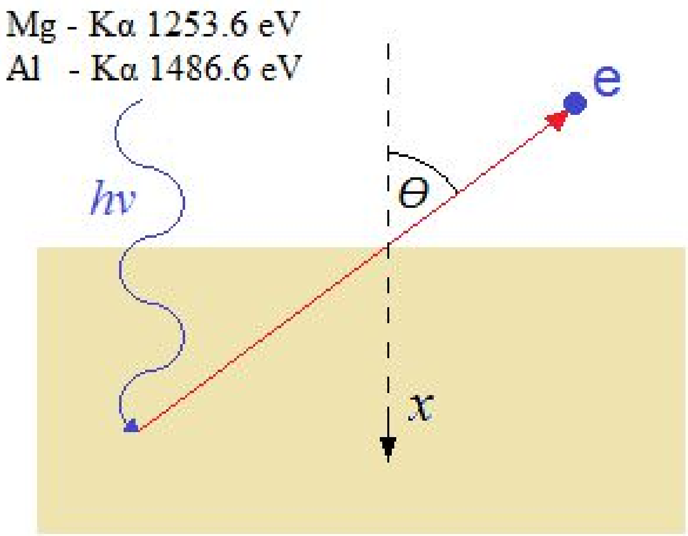
Topics and motivation

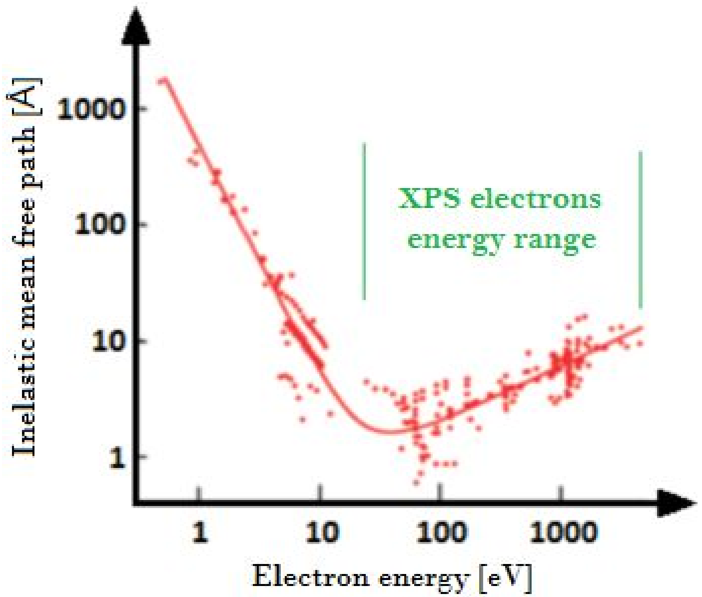
- XPS as a tool for quantitative surface analysis
- How to control graphene formation by means of XPS
- Superlattice or heterostructure quality detemination
- XPS application for quantitative analysis of graphene formation on superlattice substrate (e.g. on SiC, GaN)
- Thickness determination of an adlayer deposited on superlattice substrate

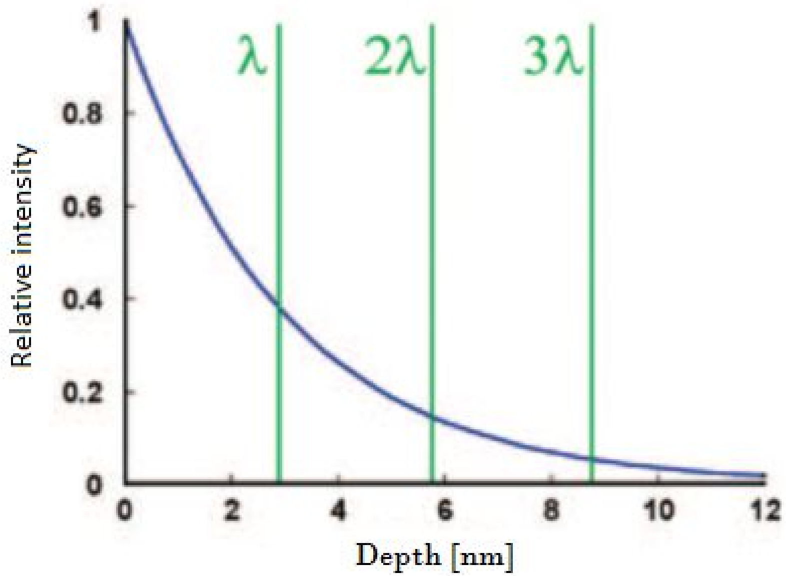
XPS and Beer-Lamberta Law



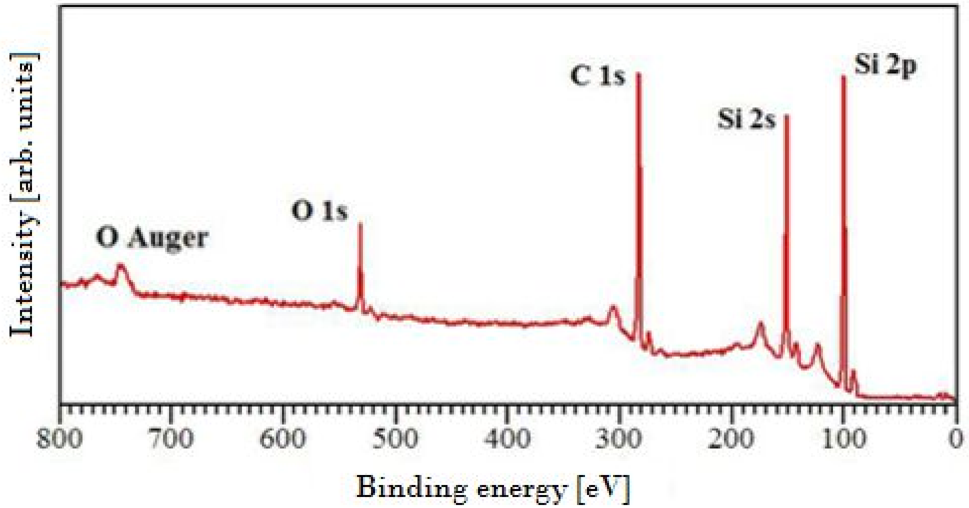
Beer-Lambert Law

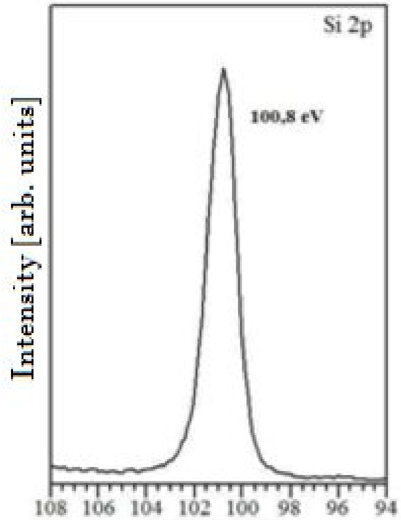
$$I(x) = I_0 \exp\left(-\frac{x}{\lambda \cos\theta}\right)$$

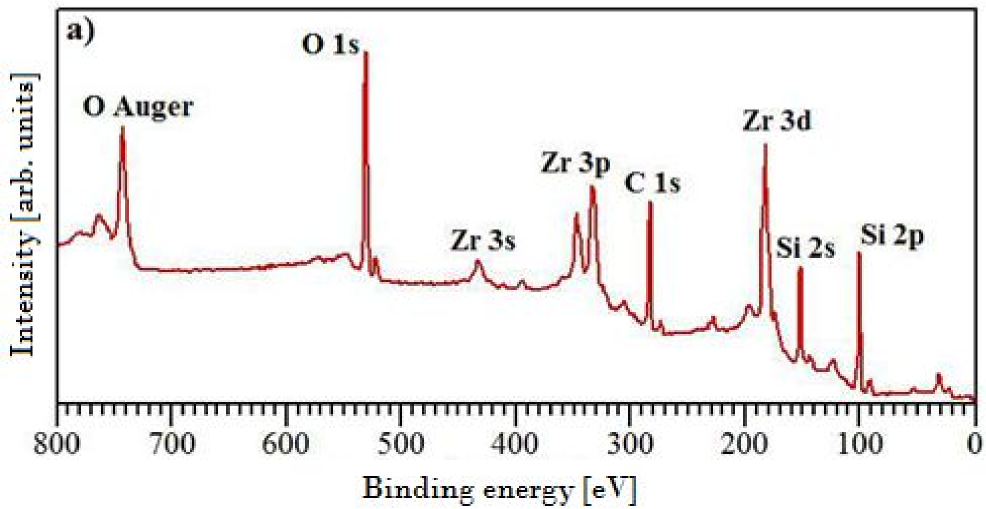


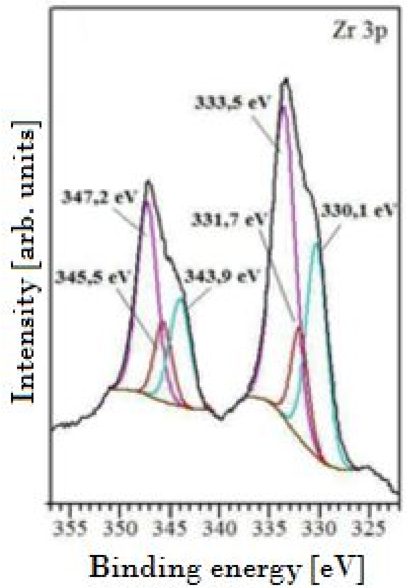


XPS



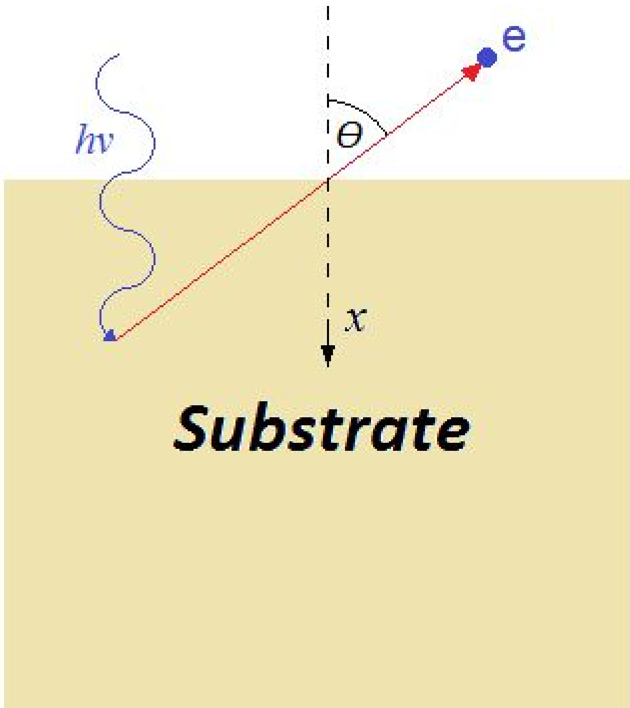






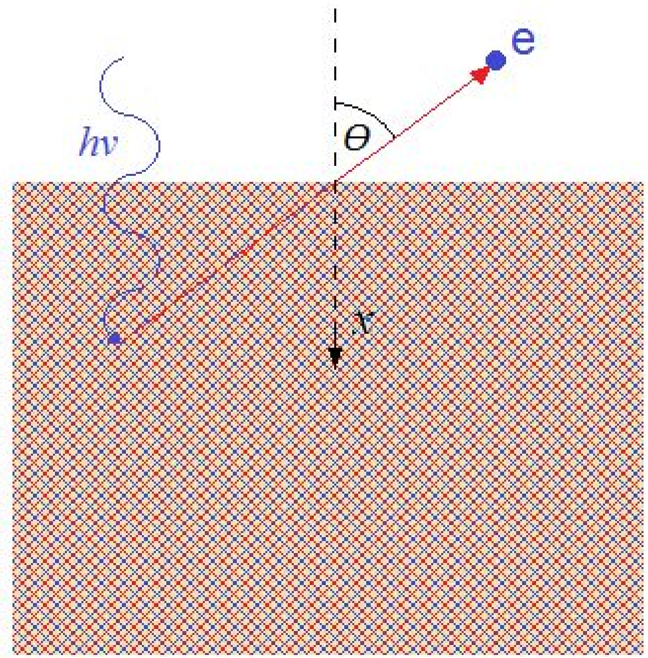
K. Idczak, Doctoral thesis, University of Wrocław 2014

XPS signal from the solid (one element only)



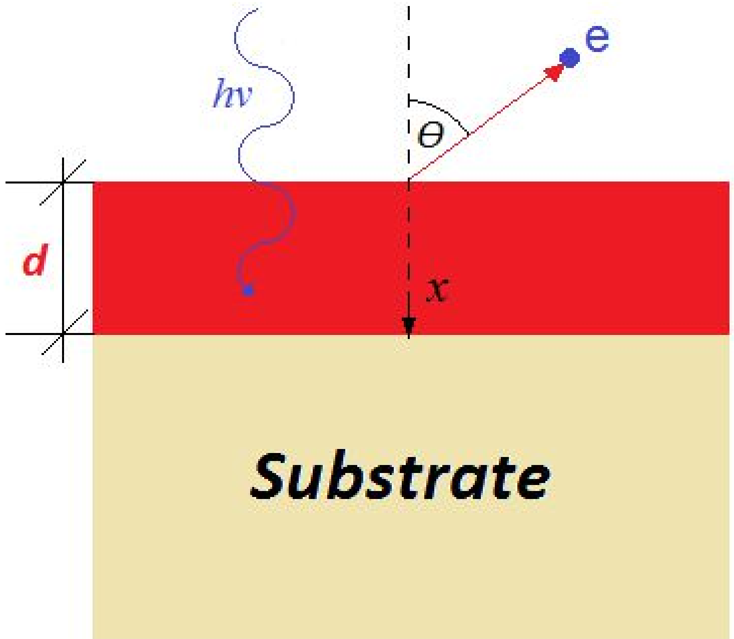
$$I_s(E_i) = k\int_0^\infty dI_s(E_i) = k\int_0^\infty n_s \sigma_s(E_i)\exp\left(-\frac{x}{\lambda_s(E_i)\cos\theta}\right)dx = kn_s\sigma_s(E_i)\lambda_s(E_i)\cos\theta$$

Atomic concentration in the solid (uniform composition)



$$n_i = \frac{\dfrac{I_i}{\sigma_i \lambda_i}}{\displaystyle\sum_{w=1}^{w=N} \frac{I_w}{\sigma_w \lambda_w}}$$

XPS signal for monoatomic adlayer deposited on a monoatomic substrate



$$\frac{I_s(E_i)}{I_{s0}(E_i)} = \exp\left(-\frac{d}{\lambda_a(E_i)\cos\theta}\right)$$

$$d = -\lambda_a(E_i)\cos\theta \ln\left[\frac{I_s(E_i)}{I_{s0}(E_i)}\right]$$

$$I_a(E_j) = k\int_0^d dI_a(E_j) = k\int_0^d n_a\sigma_a(E_j)\lambda_a(E_j)\exp\left(-\frac{x}{\lambda_a(E_j)\cos\theta}\right)dx = kn_a\sigma_a(E_j)\lambda_a(E_j)\left[1-\exp\left(-\frac{d}{\lambda_a(E_j)\cos\theta}\right)\right]$$

$$\frac{I_a(E_j)}{I_s(E_i)} = \frac{n_a\sigma_a(E_j)\lambda_a(E_j)}{n_s\sigma_s(E_i)\lambda_s(E_i)}\left[\exp\left(-\frac{d}{\lambda_a(E_i)\cos\theta}\right) - \exp\left(\frac{d}{\cos\theta}\left(\frac{1}{\lambda_a(E_i)} - \frac{1}{\lambda_a(E_j)}\right)\right)\right]$$

$$d = \lambda_a(E_i)\cos\theta\, ln\left[1 + \frac{I_a(E_j)}{I_s(E_i)}\frac{n_s\sigma_s(E_i)\lambda_s(E_i)}{n_a\sigma_a(E_j)\lambda_a(E_j)}\right]$$

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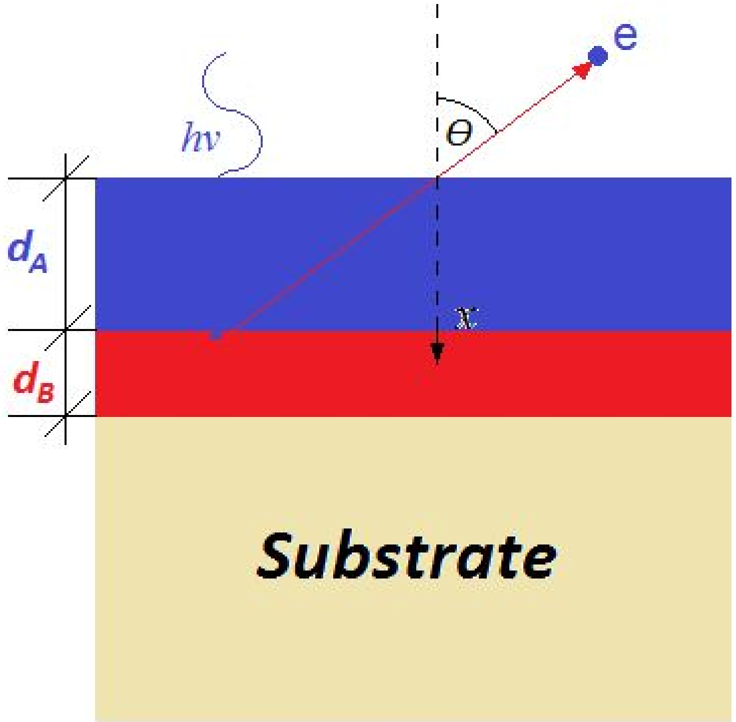
XPS signal for two monoatomic adlayers deposited on monoatomic substrate

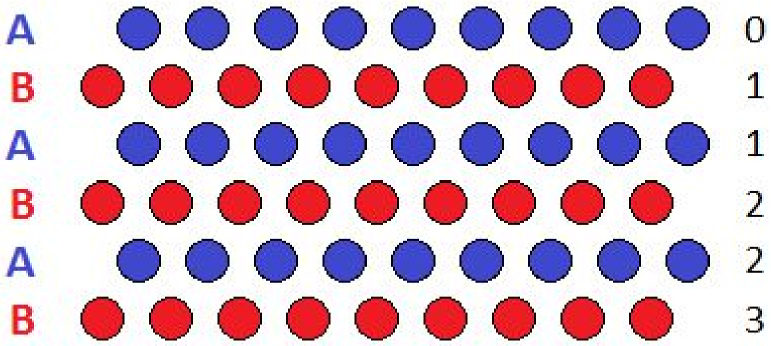


$$I_A(E_j) = kn_A\sigma_A(E_j)\lambda_A(E_j)\cos\theta \exp\left[1-\left(-\frac{d_A}{\lambda_A(E_j)\cos\theta}\right)\right]$$

$$I_B(E_l) = kn_B\sigma_B(E_l)\lambda_A(E_l)\cos\theta \exp\left[1-\left(-\frac{d_B}{\lambda_B(E_l)\cos\theta}\right)\right] * \exp\left(-\frac{d_A}{\lambda_A(E_l)\cos\theta}\right)$$

$$I_s(E_i) = kn_s\sigma_s(E_i)\lambda_s(E_i)\cos\theta \exp\left(-\frac{d_A}{\lambda_A(E_i)\cos\theta}\right) * \exp\left(-\frac{d_B}{\lambda_B(E_i)\cos\theta}\right)$$

XPS signal from crystal with two elements basis (e.g. SiC, GaN)



$$I_{A,0} = kn_A \sigma_A (E_{i,A})$$

$$I_{B,1} = kn_B \sigma_B (E_{i,B}) \exp\left(-n_A \delta_{B,A}(E_{i,B}) \cos\theta\right)$$

$$\delta_{B,B}(E_{i,B}) = \frac{1}{n_{B,bulk} \lambda_B (E_{i,B})}$$

$$I_{A,1} = kn_A \sigma_A (E_{i,A}) \exp\left(-n_B \delta_{A,B}(E_{i,A}) \cos\theta\right) \cdot \exp\left(-n_A \delta_{A,A}(E_{i,A}) \cos\theta\right)$$

$$I_{B,2} = I_{B,1} \exp\left(-n_A \delta_{B,A}(E_{i,B}) \cos\theta\right) \cdot \exp\left(-n_B \delta_{B,B}(E_{i,B}) \cos\theta\right)$$

$$I_{A,2} = I_{A,1} \exp\left(-n_B \delta_{A,B}(E_{i,A}) \cos\theta\right) \cdot \exp\left(-n_A \delta_{A,A}(E_{i,A}) \cos\theta\right)$$

$$I_{A,n} = I_{A,n-1} \exp\left(-n_B \delta_{A,B}(E_{i,A}) \cos\theta\right) \cdot \exp\left(-n_A \delta_{A,A}(E_{i,A}) \cos\theta\right)$$

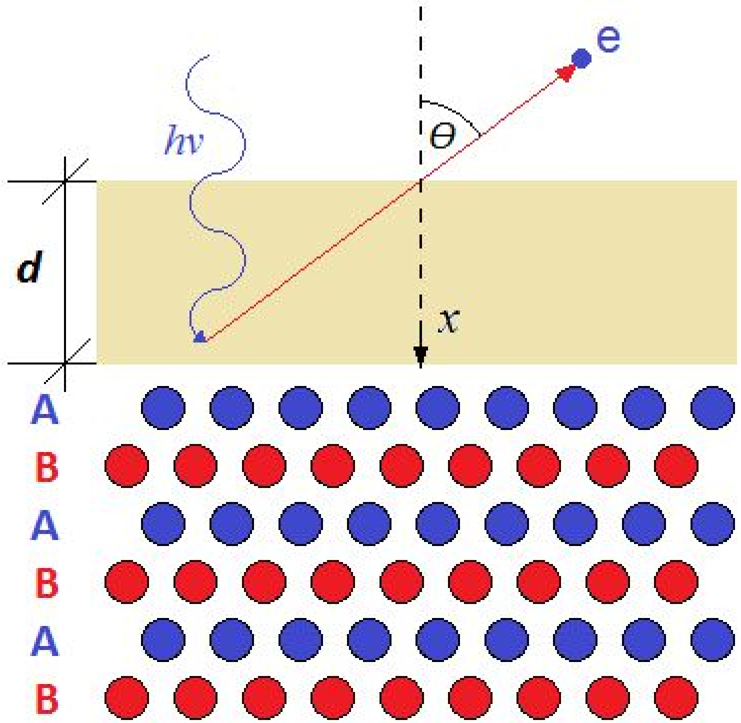
$$I_{B,n} = I_{B,n-1} \exp\left(-n_A \delta_{B,A}(E_{i,B}) \cos\theta\right) \cdot \exp\left(-n_B \delta_{B,B}(E_{i,B}) \cos\theta\right)$$

$$\sum_{n=1}^{\infty} aq^{n-1} = \frac{a}{1-q}$$

$$I_A = \sum_{n=0}^{\infty} I_{A,n} = \frac{I_{A,0}}{1 - \exp\left(-n_B \delta_{A,B}(E_{i,A}) \cos\theta\right) \cdot \exp\left(-n_A \delta_{A,A}(E_{i,A}) \cos\theta\right)}$$

$$I_B = \sum_{n=1}^{\infty} I_{B,n} = \frac{I_{B,1}}{1 - \exp\left(-n_A \delta_{B,A}(E_{i,A}) \cos\theta\right) \cdot \exp\left(-n_B \delta_{B,B}(E_{i,B}) \cos\theta\right)}$$

XPS signal for monoatomic adlayer deposited on two-elements crystal



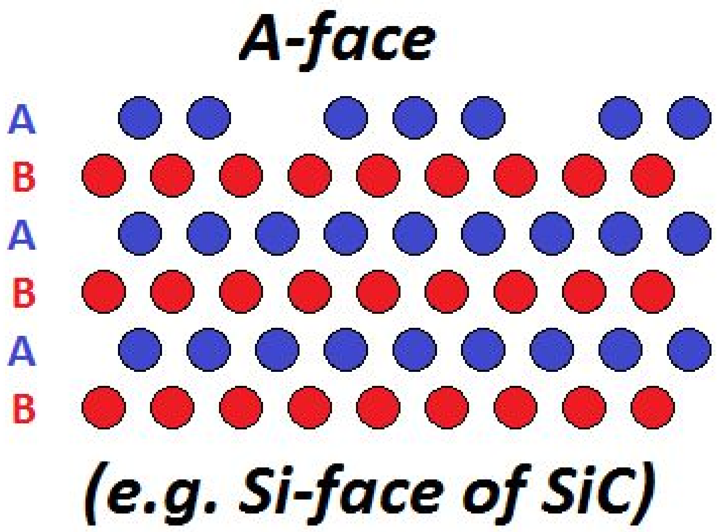
$$I_a(E_j) = kn_a\sigma_a(E_j)\lambda_a(E_j)\left[1-\exp\left(-\frac{d}{\lambda_a(E_j)\cos\theta}\right)\right]$$

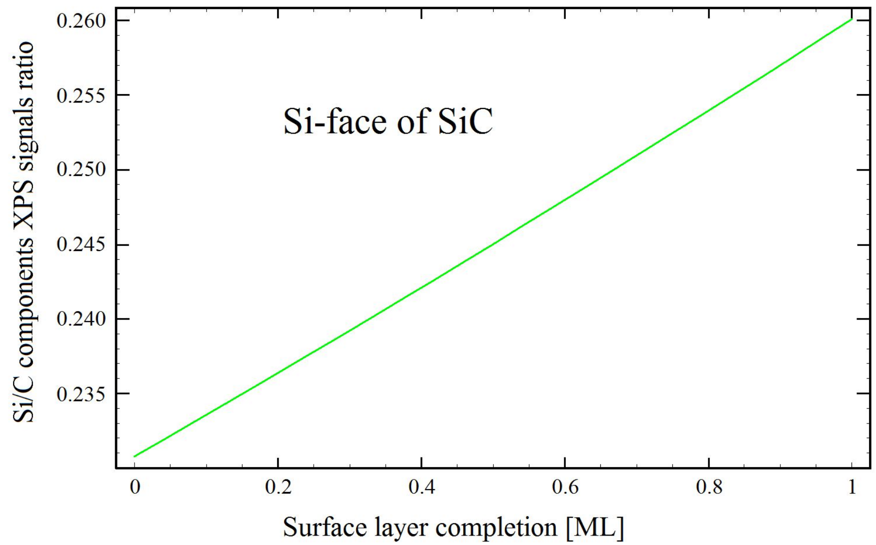
$$I_{Aa} = I_A\cos\theta\exp\left(-\frac{d}{\lambda_a(E_{i,A})\cos\theta}\right)$$

$$I_{Ba} = I_B\cos\theta\exp\left(-\frac{d}{\lambda_a(E_{i,B})\cos\theta}\right)$$

$$\frac{I_a(E_j)}{I_{Aa}(E_{i,A})} = \frac{n_a\sigma_a(E_j)\lambda_a(E_j)}{n_A\sigma_A(E_{i,A})}\left[1-\exp\left(-\frac{d}{\lambda_a(E_j)\cos\theta}\right)\right]\left[1-\exp\left(-n_B\delta_{A,B}(E_{i,A})\cos\theta\right)\cdot\exp\left(-n_A\delta_{A,A}(E_{i,A})\cos\theta\right)\right]$$

XPS signal from two-elements crystal during surface layer decomposition





$$I_{A,0} = Pkn_A\sigma_A(E_{i,A})$$

P - first layer filling coefficient

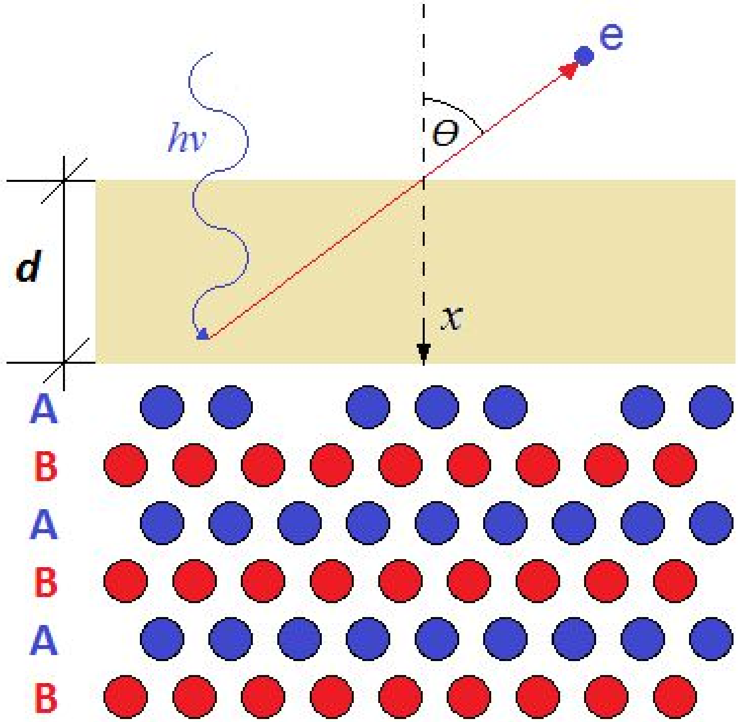
$$I_{B,1} = kn_B\sigma_B(E_{i,B})\exp\left(-Pn_A\delta_{B,A}(E_{i,B})\cos\theta\right)$$

$$I_{A,1} = kn_A\sigma_A(E_{i,A})\exp\left(-n_B\delta_{A,B}(E_{i,A})\cos\theta\right)\cdot\exp\left(-Pn_A\delta_{A,A}(E_{i,A})\cos\theta\right)$$

$$I_A = \sum_{n=1}^{\infty} I_{A,n} = \frac{I_{A,1}}{1-\exp\left(-n_B\delta_{A,B}(E_{i,A})\cos\theta\right)\cdot\exp\left(-n_A\delta_{A,A}(E_{i,A})\cos\theta\right)} + I_{A,0}$$

$$I_B = \sum_{n=1}^{\infty} I_{B,1} = \frac{I_{B,1}}{1-\exp\left(-n_A\delta_{B,A}(E_{i,A})\cos\theta\right)\cdot\exp\left(-n_B\delta_{B,B}(E_{i,B})\cos\theta\right)}$$

XPS signal for monoatomic adlayer deposited on two-elements crystal with incomplete surface layer



$$\frac{I_a(E_j)}{I_{Ba}(E_{i,B})} = \frac{n_a \sigma_a(E_j)\lambda_a}{n_B \sigma_B(E_{i,B})}\left[1-\exp\left(-\frac{d}{\lambda_a(E_j)\cos\theta}\right)\right]$$
$$\left[1-\exp\left(-n_A\delta_{B,A}(E_{i,A})\cos\theta\right)\cdot\exp\left(-n_B\delta_{B,B}(E_{i,B})\cos\theta\right)\right]\exp\left(Pn_A\delta_{B,A}(E_{i,B})\cos\theta\right)$$

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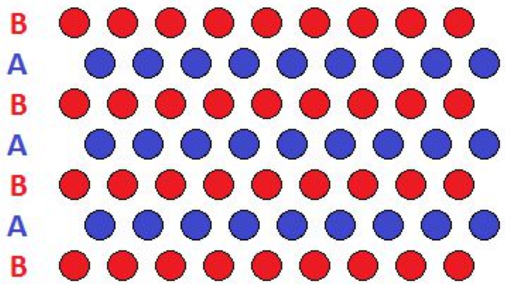
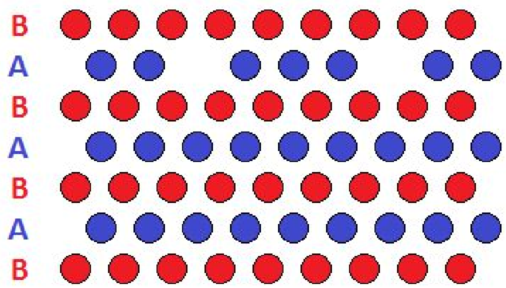
Surface bilayer formation on two-elements crystal (e.g. graphene on SiC)

B-face



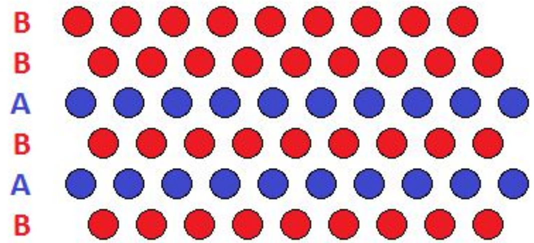
(e.g. C-face of SiC)

B-face



(e.g. C-face of SiC)

surface bilayer



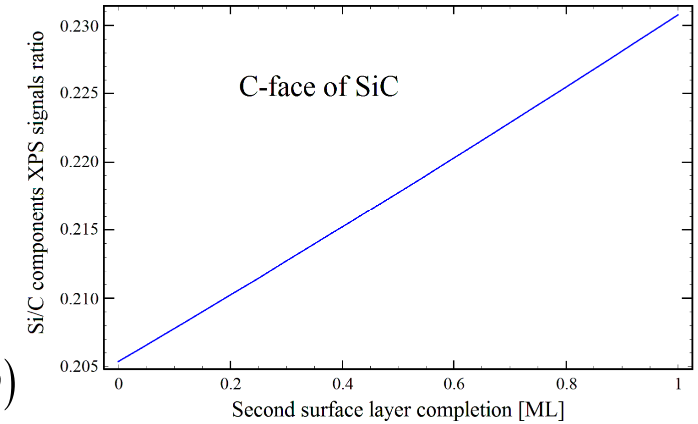
(e.g. graphene on SiC)

$$I_{B,0} = kn_B\sigma_B(E_{i,B})$$

$$I_{A,1} = Pkn_A\sigma_A(E_{i,A})\exp\left(-n_B\delta_{A,B}(E_{i,A})\cos\theta\right)$$

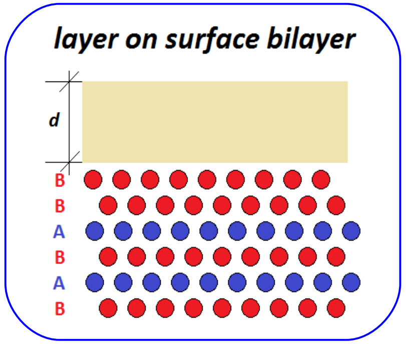
$$I_{B,1} = kn_B\sigma_B(E_{i,B})\exp\left(-Pn_A\delta_{B,A}(E_{i,B})\right)\cdot\exp\left(-n_B\delta_{B,B}(E_{i,B})\right)$$

$$I_{A,2} = \frac{I_{A,1}}{P}\exp\left(-n_B\delta_{A,B}(E_{i,A})\cos\theta\right)\cdot\exp\left(-Pn_A\delta_{A,A}(E_{i,A})\cos\theta\right)$$



$$I_B = \sum_{n=1}^{\infty} I_{B,n} = \frac{I_{B,1}}{1-\exp\left(-n_A\delta_{B,A}(E_{i,B})\cos\theta\right)\cdot\exp\left(-n_B\delta_{B,B}(E_{i,B})\cos\theta\right)} + I_{B,0}$$

$$I_A = \sum_{n=2}^{\infty} I_{A,n} = \frac{I_{A,2}}{1-\exp\left(-n_B\delta_{A,B}(E_{i,B})\cos\theta\right)\cdot\exp\left(-n_A\delta_{A,A}(E_{i,A})\cos\theta\right)} + I_{A,1}$$



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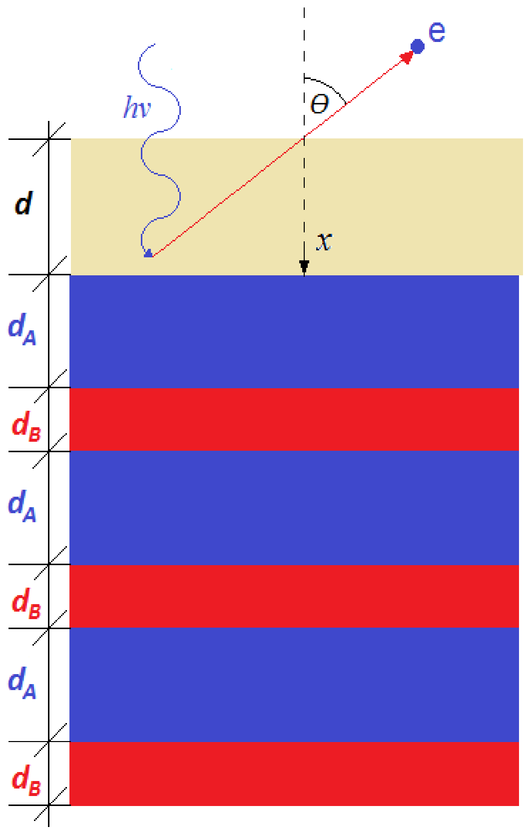
Thickness determination of an adlayer deposited on superlattice substrate

adlayer on superlattice



$$\frac{I_a(E_j)}{I_{Aa}(E_{i,A})}=\frac{n_a\,\sigma_a(E_j)\,\lambda_a}{n_{A,bulk}\,\sigma_A(E_{i,A})\,\lambda_a(E_{i,A})}\left[\frac{1-\exp\left(-\frac{d}{\lambda_a(E_j)\cos\theta}\right)}{1-\exp\left(-\frac{d_A}{\lambda_A(E_{i,A})\cos\theta}\right)}\right]\left[1-\exp\left(-\frac{d_B}{\lambda_B(E_{i,A})\cos\theta}\right)\exp\left(-\frac{d_A}{\lambda_A(E_{i,A})\cos\theta}\right)\right]$$

Thank you for your attention!