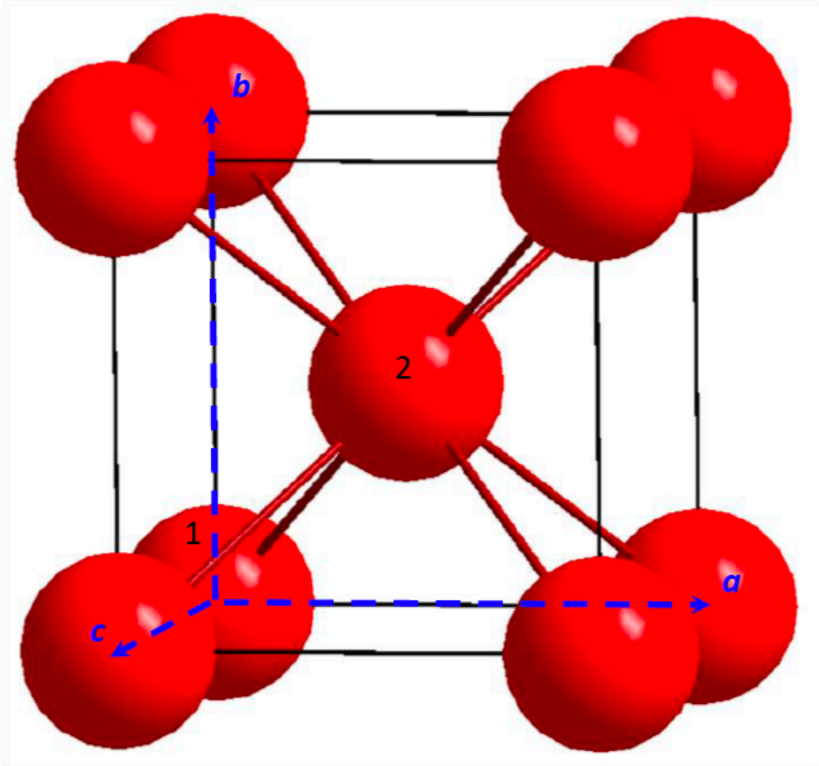
FZM 419

4

Örnek: Hacim merkezli kübik (BCC) yapı



$$a = b = c$$

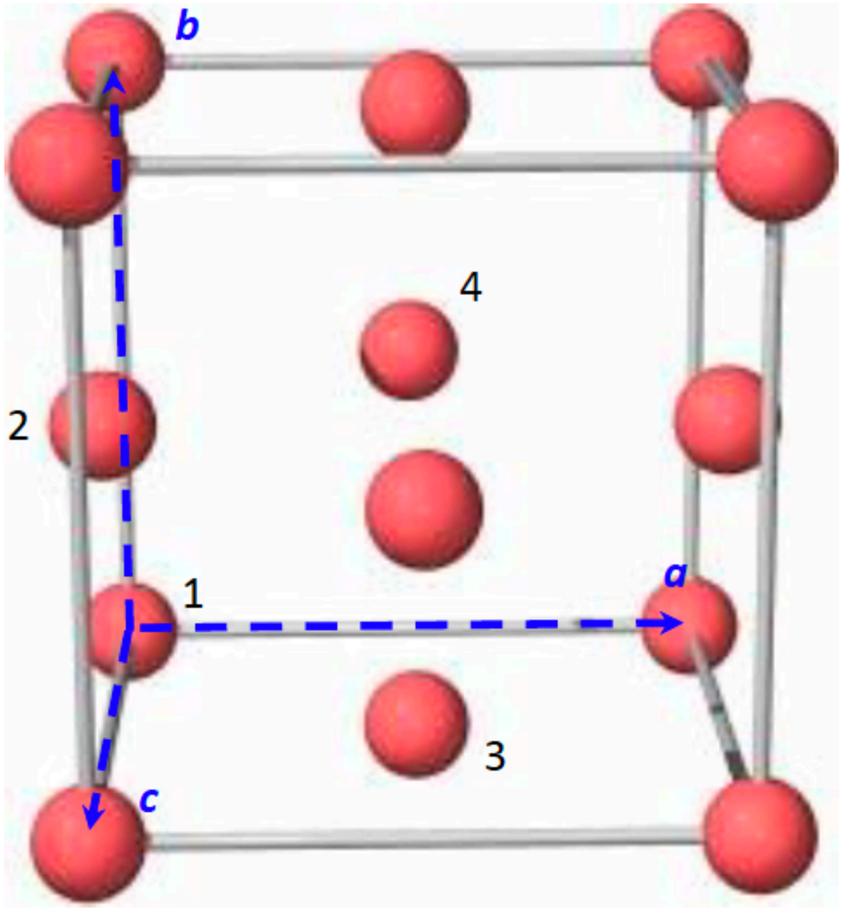
$$\alpha = \beta = \gamma = 90$$

$$\boldsymbol{R_1} = [000]$$

$$\boldsymbol{R_2} = [\frac{1}{2}\frac{1}{2}\frac{1}{2}]$$

Two atoms per unit cell

Örnek: Yüzey merkezli kübik (BCC) yapı



$a = b = c$

$\alpha = \beta = \gamma = 90$

$\boldsymbol{R_1} = [0\ 0\ 0]$

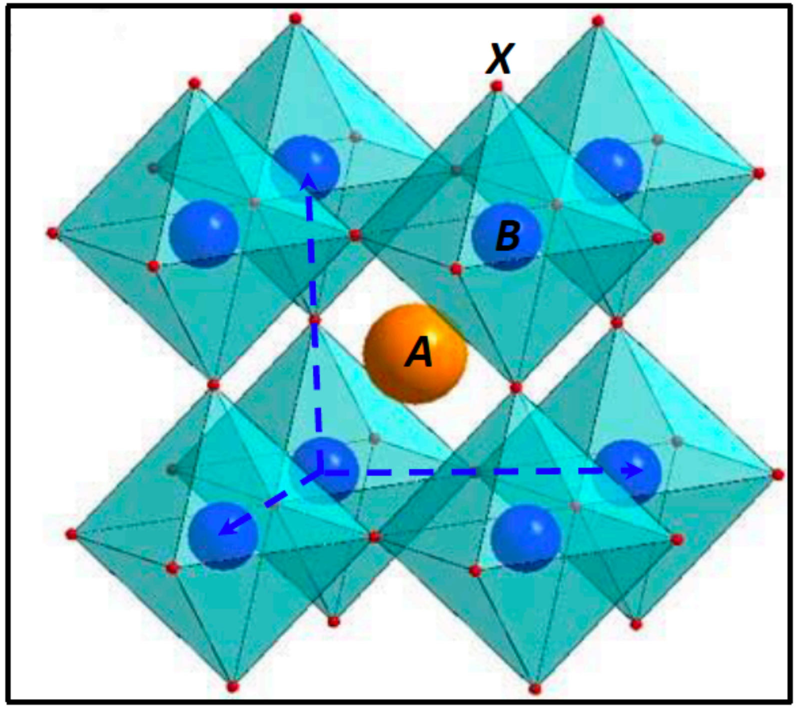
$\boldsymbol{R_2} = [0\ \frac{1}{2}\ \frac{1}{2}]$

$\boldsymbol{R_3} = [\frac{1}{2}\ 0\ \frac{1}{2}]$

$\boldsymbol{R_4} = [\frac{1}{2}\ \frac{1}{2}\ 0]$

4 atoms per unit cell

Örnek: KÜBİK PEROVSKITE, ABO3



5 atoms per unit cell

$a = b = c$

$\alpha = \beta = \gamma = 90$

$$R_B = [0\ 0\ 0]$$

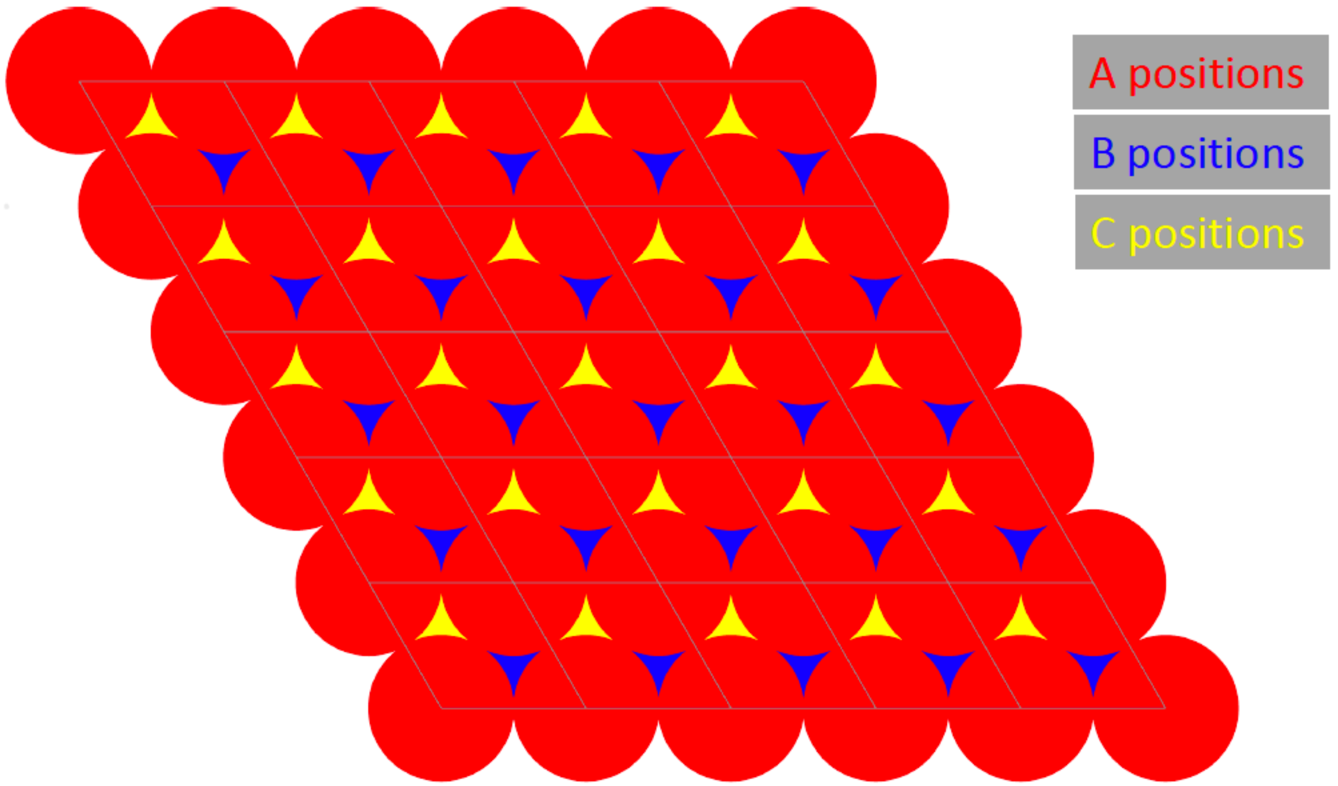
$$R_A = [\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}]$$

$$R_{X1} = [\tfrac{1}{2}\ 0\ 0]$$

$$R_{X2} = [0\ \tfrac{1}{2}\ 0]$$

$$R_{X3} = [0 0\ \tfrac{1}{2}]$$

Hexagonal close packing (HCP)

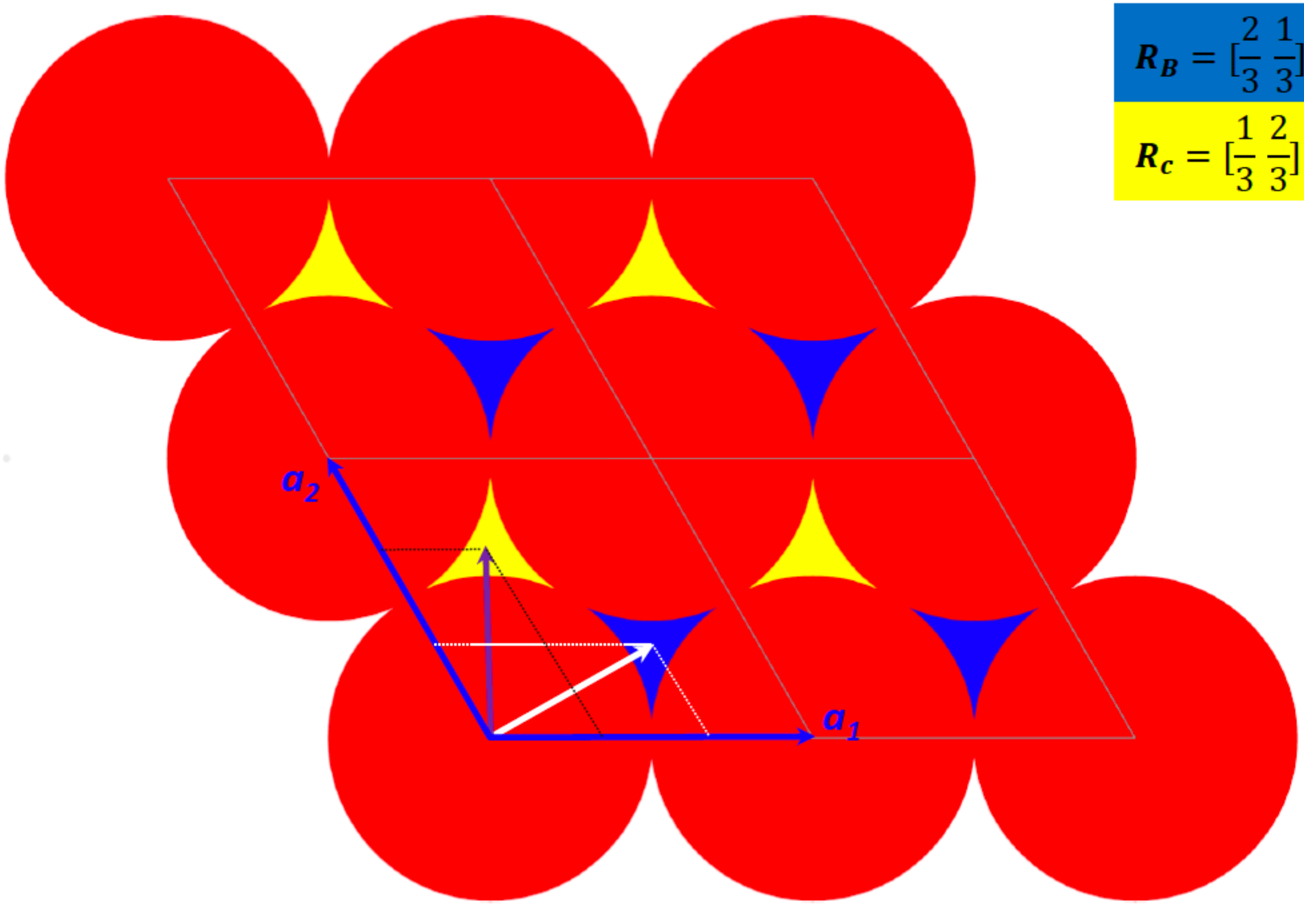


HCP positions

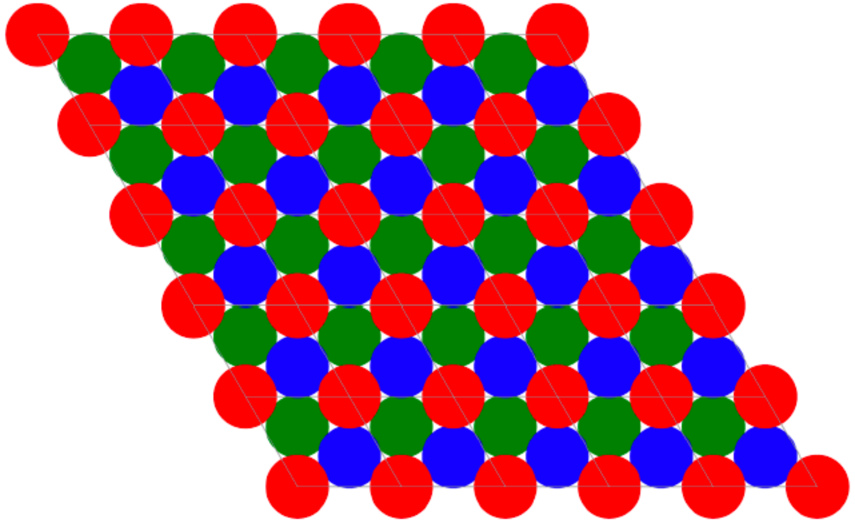
$R_A = [00]$

$R_B = [\frac{2}{3}\frac{1}{3}]$

$R_c = [\frac{1}{3}\frac{2}{3}]$



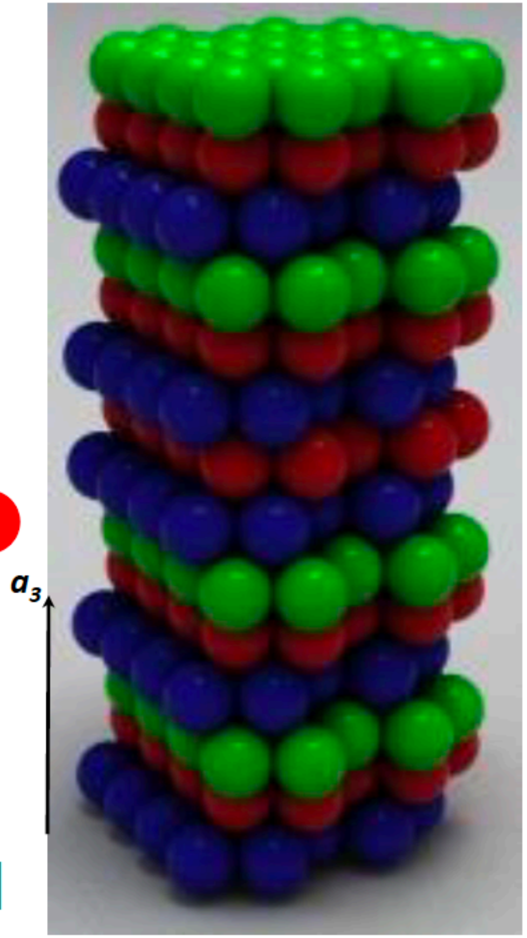
Three dimensional HCP structure



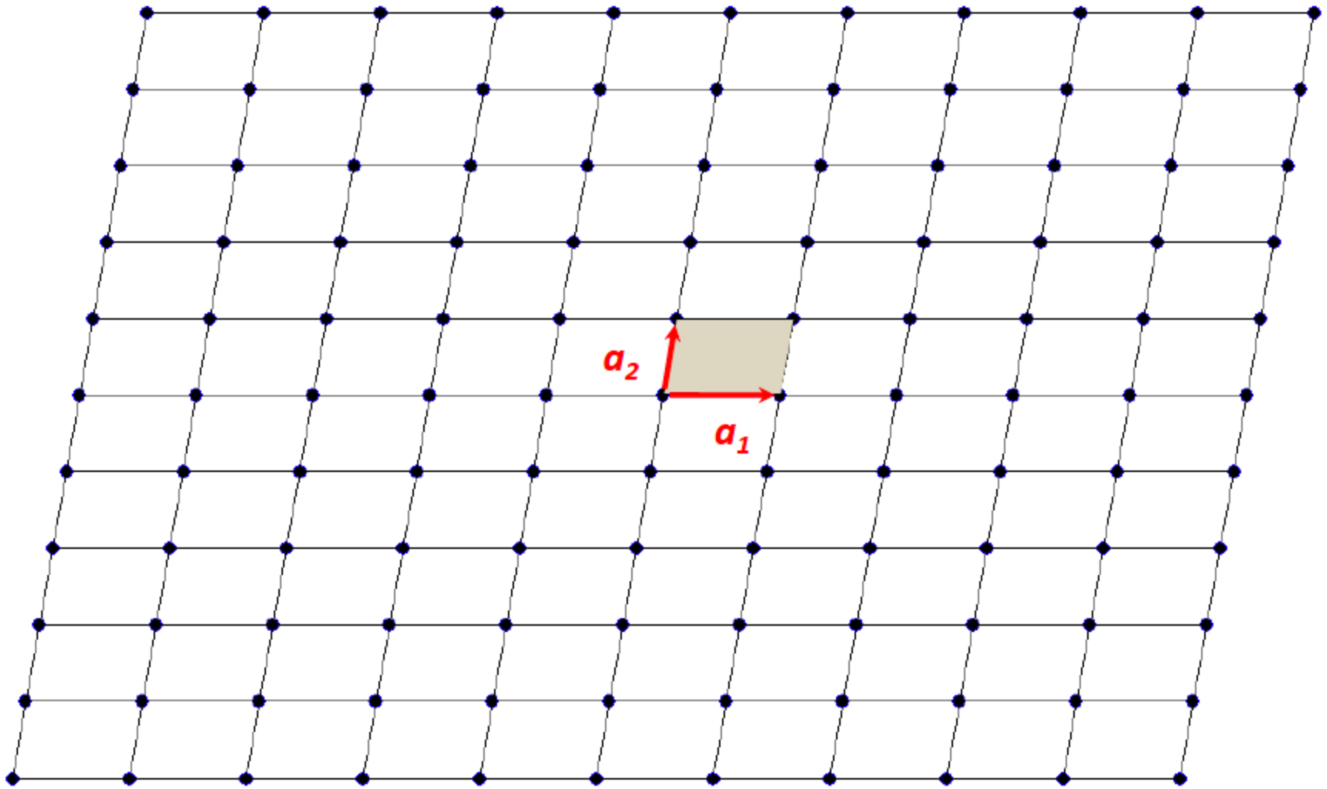
$$R_A = [000]$$

$$R_B = [\frac{2}{3}\,\frac{1}{3}\,\frac{1}{3}]$$

$$R_c = [\frac{1}{3}\,\frac{2}{3}\,\frac{2}{3}]$$



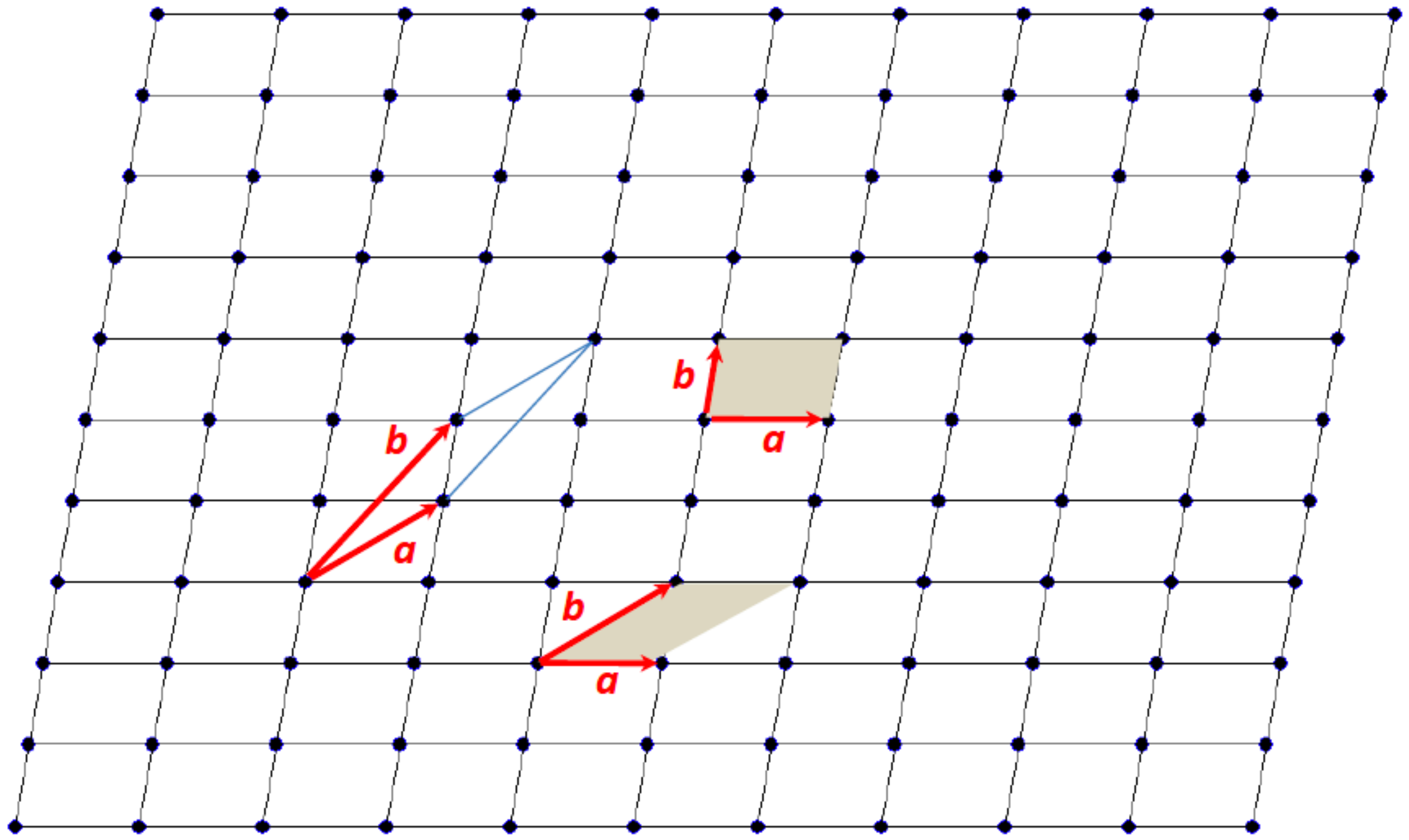
BAZ VEKTÖRLERi ve KRİSTAL ÖRGÜ PARAMETRELERİ



Lattice parameters for two dimensional case: $a=|\boldsymbol{a}|$, $b=|\boldsymbol{b}|$, $\alpha=\angle(\boldsymbol{a},\boldsymbol{b})$

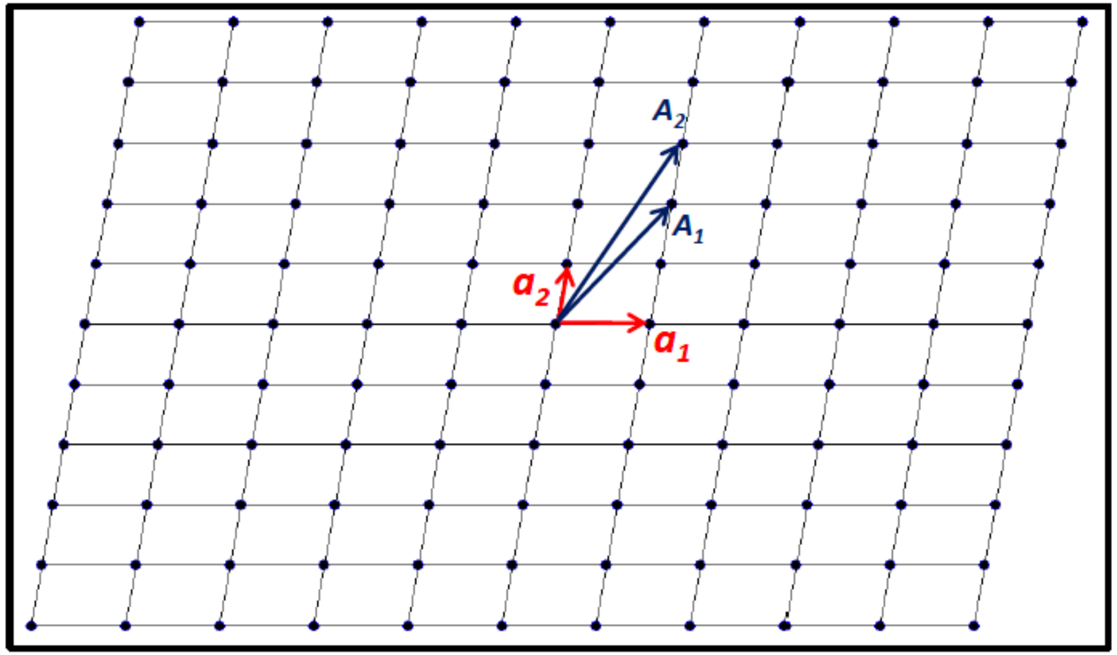
For the given example: a=1.5, b=1, α=80 deg

Farklı baz vektörleri ve kafes parametreleri seçenekleri



Kafes baz vektörlerinin ve dolayısıyla kafes parametrelerinin seçim özgürlüğü vardır.

Baz vektörlerin seçimi hakkında teorem



A1 ve a2 olmak üzere iki baz vektör ile oluşturulan kafesi düşünün
Diğer iki kafes vektörü alın

$$A_1=[u_{1i}]=u_{11}\boldsymbol{a_1}+u_{12}\boldsymbol{a_2}$$
$$A_2=[u_{2i}]=u_{21}\boldsymbol{a_1}+u_{22}\boldsymbol{a_2}$$

u_{ij} tam sayıdır

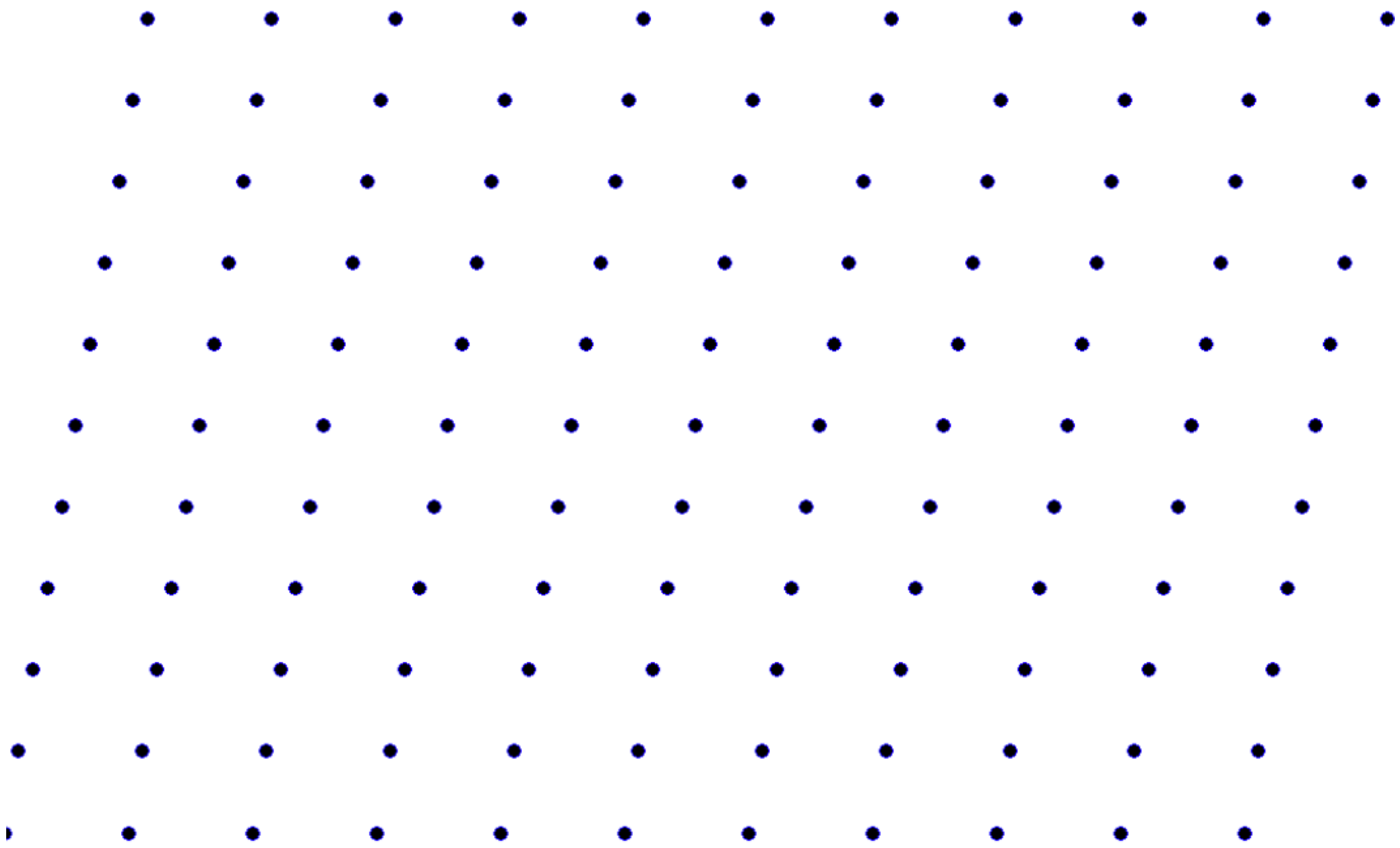
Bu yeni vektör çifti aynı kafesi mi oluşturuyor ?

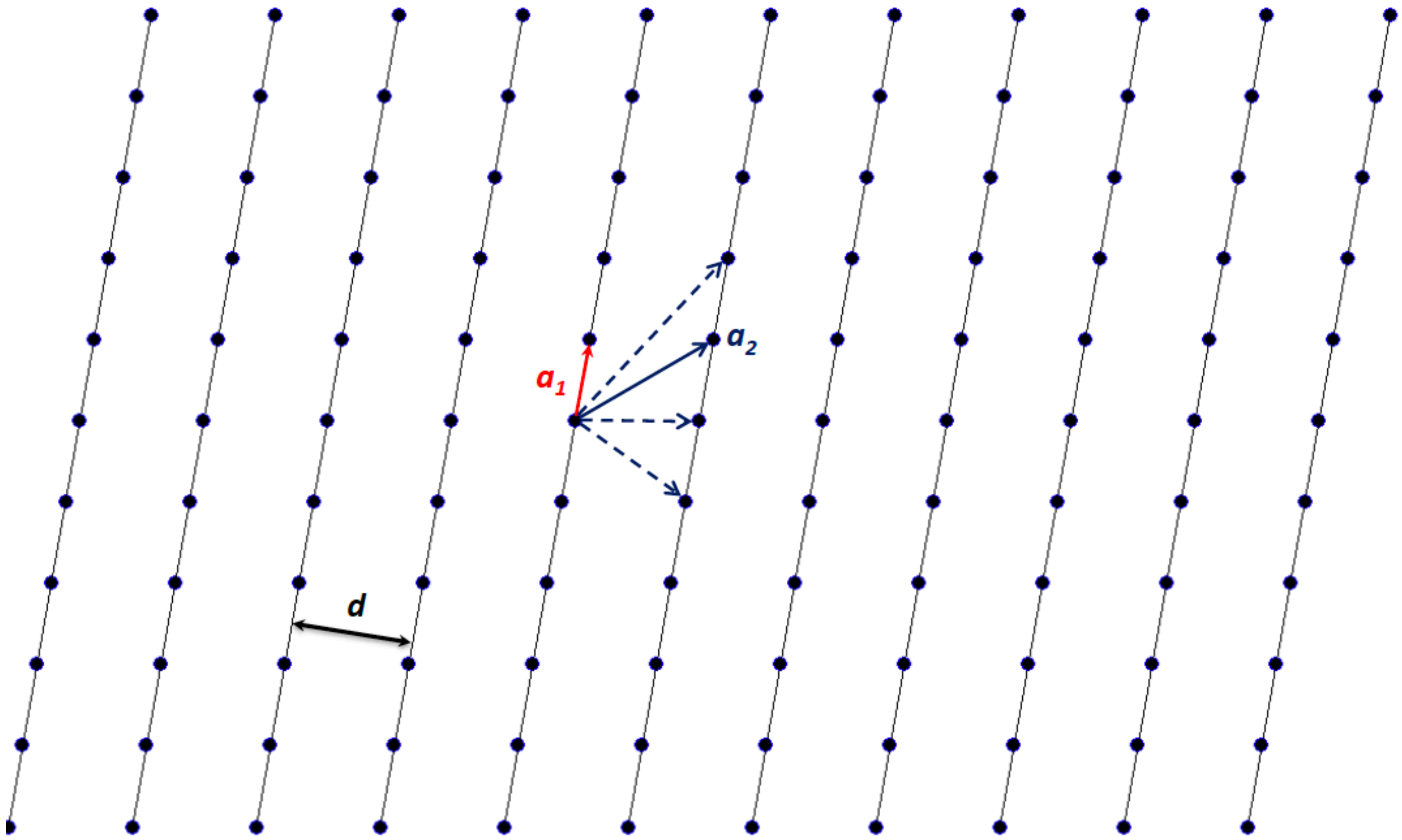
A1 ve a2 üzerine inşa edilen paralelkenarın alanı S'nin aynı olmasını sağlamak gerekir.
A1 ve A2 üzerine inşa edilen paralelkenar alanı olarak

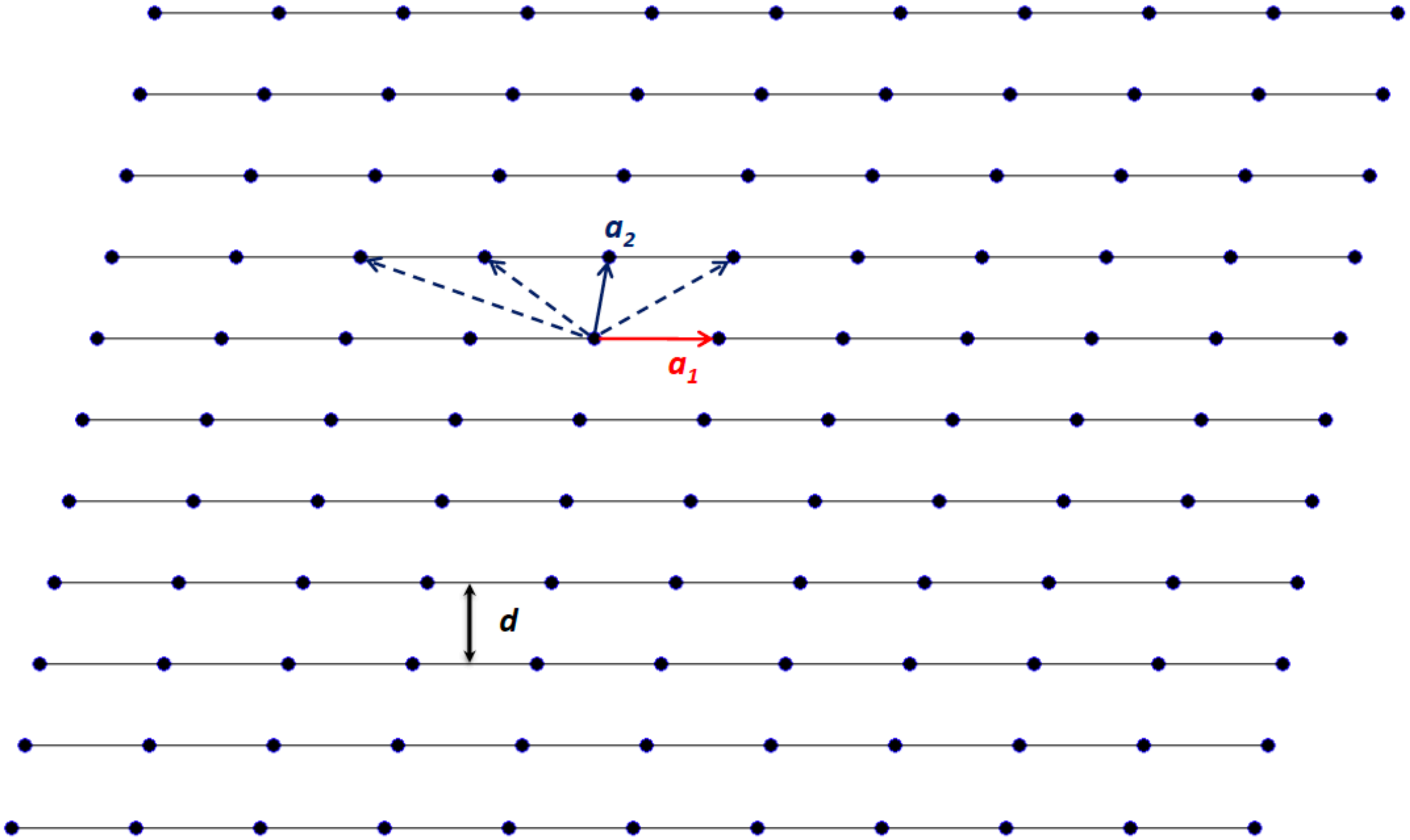
$$S(\boldsymbol{A_1}, \boldsymbol{A_2}) = \pm \begin{vmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{vmatrix} S(\boldsymbol{a_1}, \boldsymbol{a_2}) \qquad \begin{vmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{vmatrix} = \pm 1$$

Son denklem A1 ve A2 vektör çifti için sağlanırsa, aynı kafes için baz vektörleri olarak seçilebilir

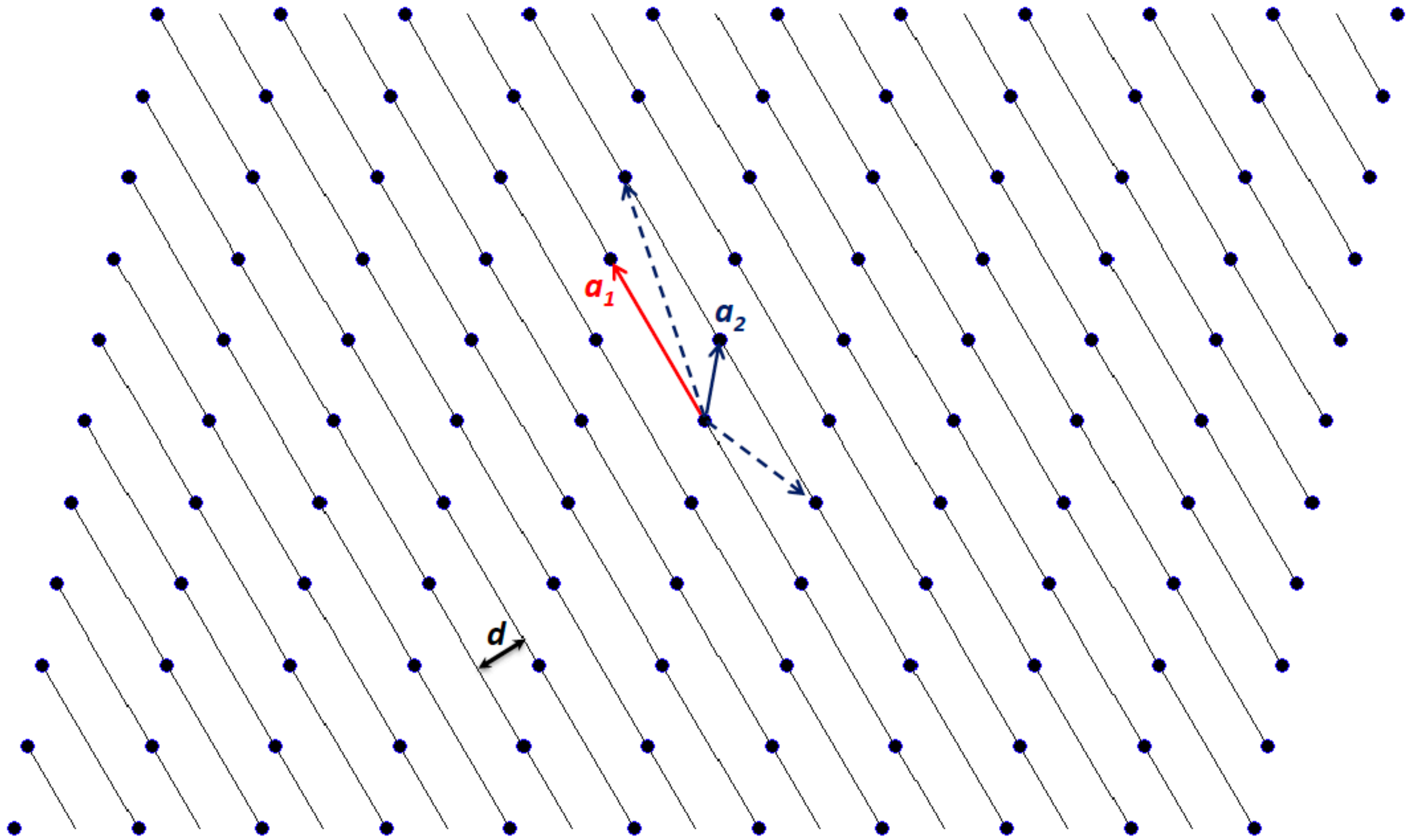
Örgü sıraları (2D) / Kafes düzlemleri (3D)



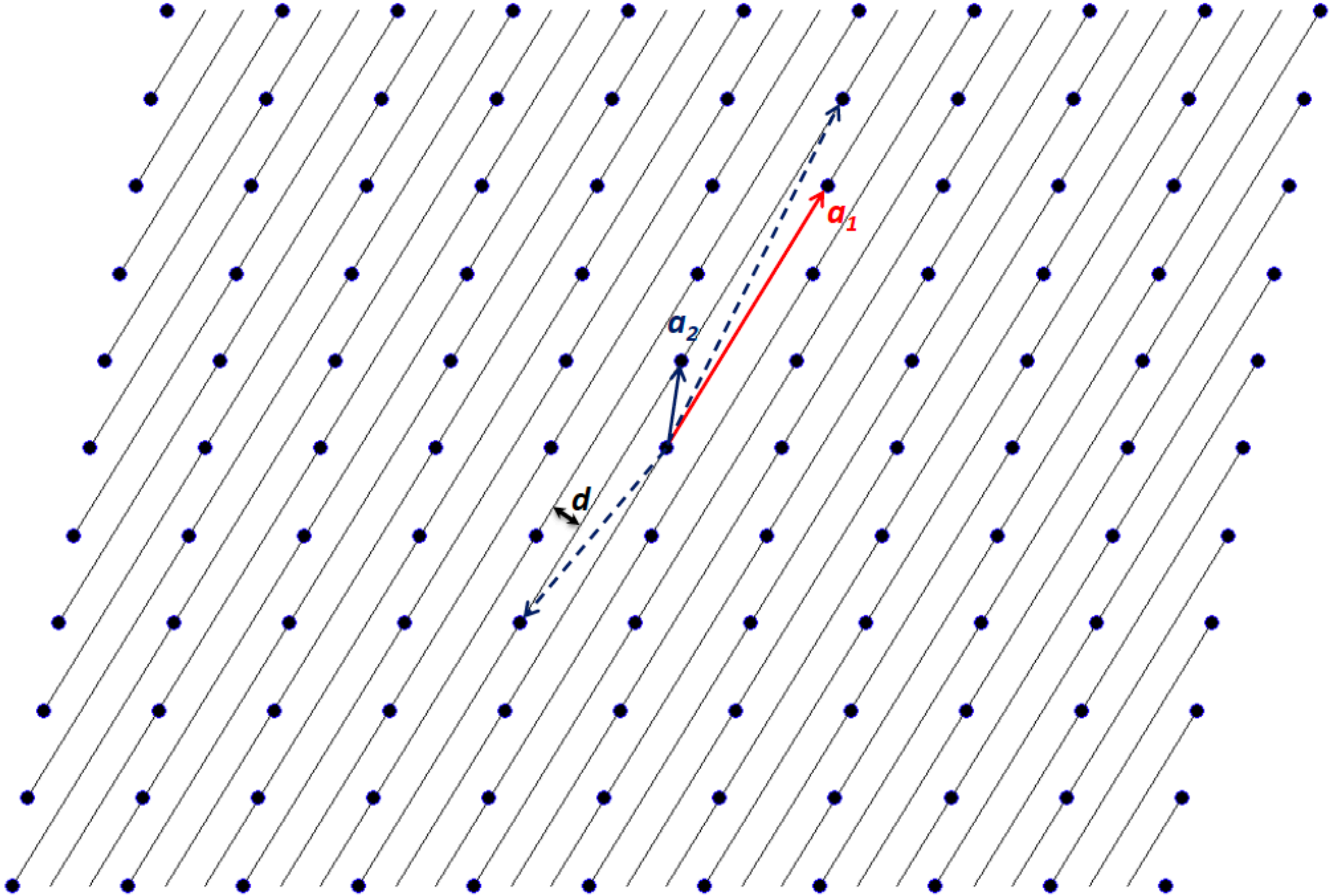

a₁
a₂
d



a2
a1
d



a_1
a_2
d



a_1
a_2
d