UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

# Crystallography (*winter term 2015/2016*)

**Lecturer:** **Dr Semën Gorfman (**ENC B-011)

**Exercise tutor:** **Hyeokmin Choe** **(**ENC B-015)

## Exercise sheet 1: Crystal lattice, lattice planes and Miller indices

Crystal lattice is a mathematical object, representing translational long-range order in crystals. It contains an infinite number of points, whose positions are $u_i \boldsymbol{a}_i$ with $u_i$ are all integer numbers. However, the choice of lattice basis vectors is not unique: the same lattice can be "generated" any another three vectors $\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{A}_3$ ($\boldsymbol{A}_i = u_{ij}\boldsymbol{a}_j$) if

$$\begin{vmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{vmatrix} = \pm 1 \text{ (3D case)} \qquad \begin{vmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{vmatrix} = \pm 1 \quad \text{(2D case)} \quad (*)$$

This means that the parameters (a, b, c, α, β, γ) are also not unique. In the two following tasks you will find three alternative sets of lattice parameters to the ones originally given. You must choose alternative (pairs) triples of basis vectors, which are compatible with (*). After that, you would calculate the corresponding new lattice parameters according to (3D case)

$$a_{new} = A_1 \qquad b_{new} = A_2 \qquad c_{new} = A_3$$
$$\alpha_{new} = \angle(\boldsymbol{A}_2, \boldsymbol{A}_3) \quad \beta_{new} = \angle(\boldsymbol{A}_1, \boldsymbol{A}_3) \quad \gamma_{new} = \angle(\boldsymbol{A}_1, \boldsymbol{A}_2)$$

### 1. 2D lattice (6 points)

The lattice parameters of a two-dimensional crystal are $a = b = 5\ A$, $\alpha = 120°$. Find three alternatives, which describe exactly the same lattice. Write the coordinates of the new basis vectors.

UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

**2. 3D lattice (9 points)**

3D crystal lattice parameters are given $a = b = 5\ A$, c = 6 A $\alpha = \beta = \gamma = 90°$. Find any three alternatives for the parameters of the same lattice. Write the coordinates of the new basis vectors.

**3. Reciprocal basis vectors (6 points)**

Explain the meaning of the reciprocal basis and the mathematical reason for its introducing? Plot the direct, $\{\boldsymbol{a}_i\}$ and reciprocal $\{\boldsymbol{a}_i^*\}$ basis for the lattices, with the following parameters: a) a = 5, b = 5, $\alpha$= 90° b) a = 5, b = 5, $\alpha$ = 120° c) a = 7, b = 8, $\alpha$= 105°. Calculate the reciprocal lattice parameters.

**4. Miller indices and lattice planes (6 points)**

Give the Miller indices for the lattice planes presented in Fig 1 (a,b,c,d). Explain your choice. (Define the pair of basis vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ by yourself)

**5. Miller indices and lattice planes (6 points)**

Plot the set of 2D lattice planes / rows with the Miller indices:

a) (1 0); b) (3 -1); c) (2 1); d) (4 1); e) (-1 6); f) (3 5);

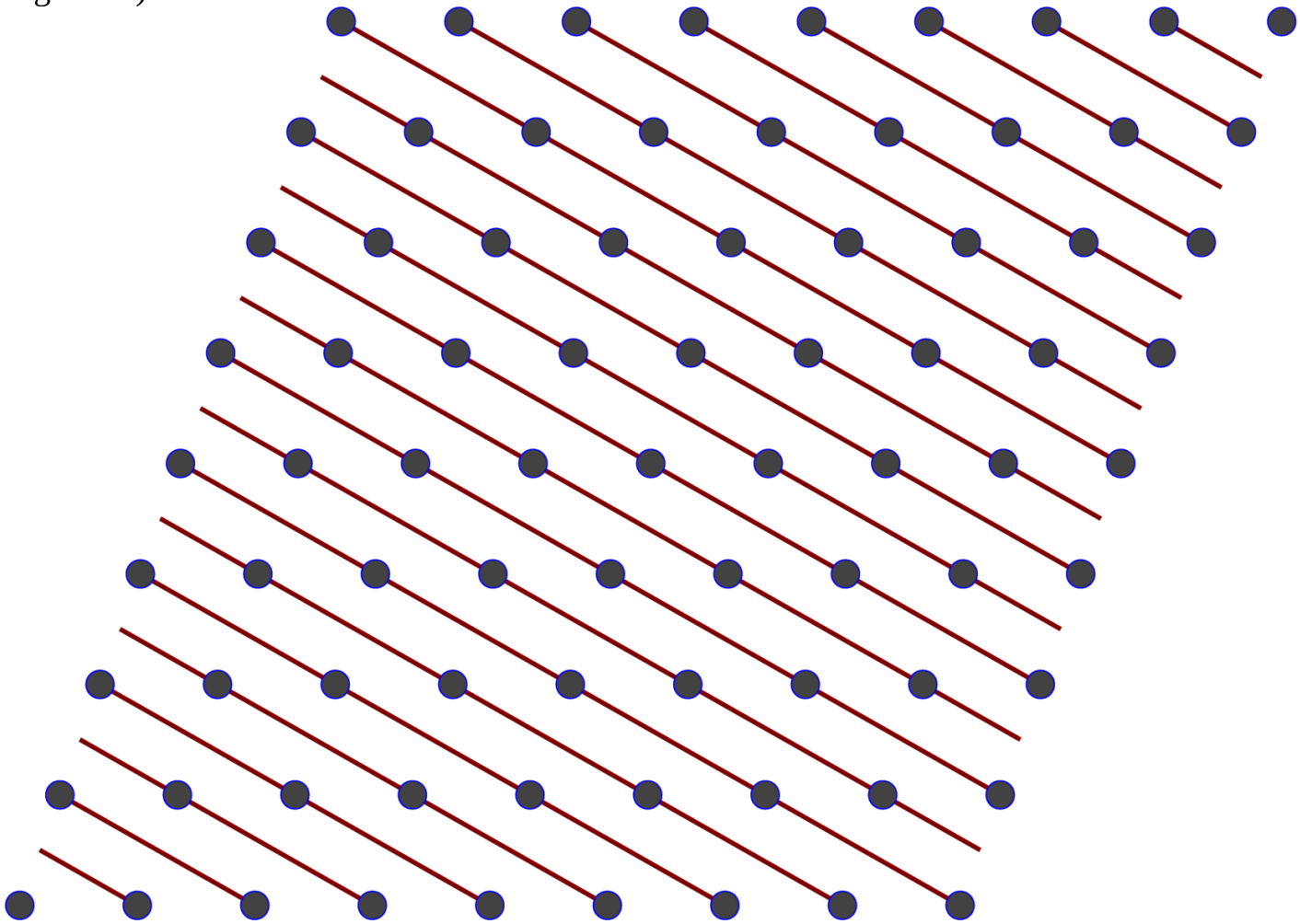
The lattices (ready to print) are given in the supplementary file (download from the course web-site). (Define the pair of basis vectors $a_1$ and $a_2$ by yourself)

Please return on 16/11/2015

UNIVERSITÄT SIEGEN

FESTKÖRPERPHYSIK

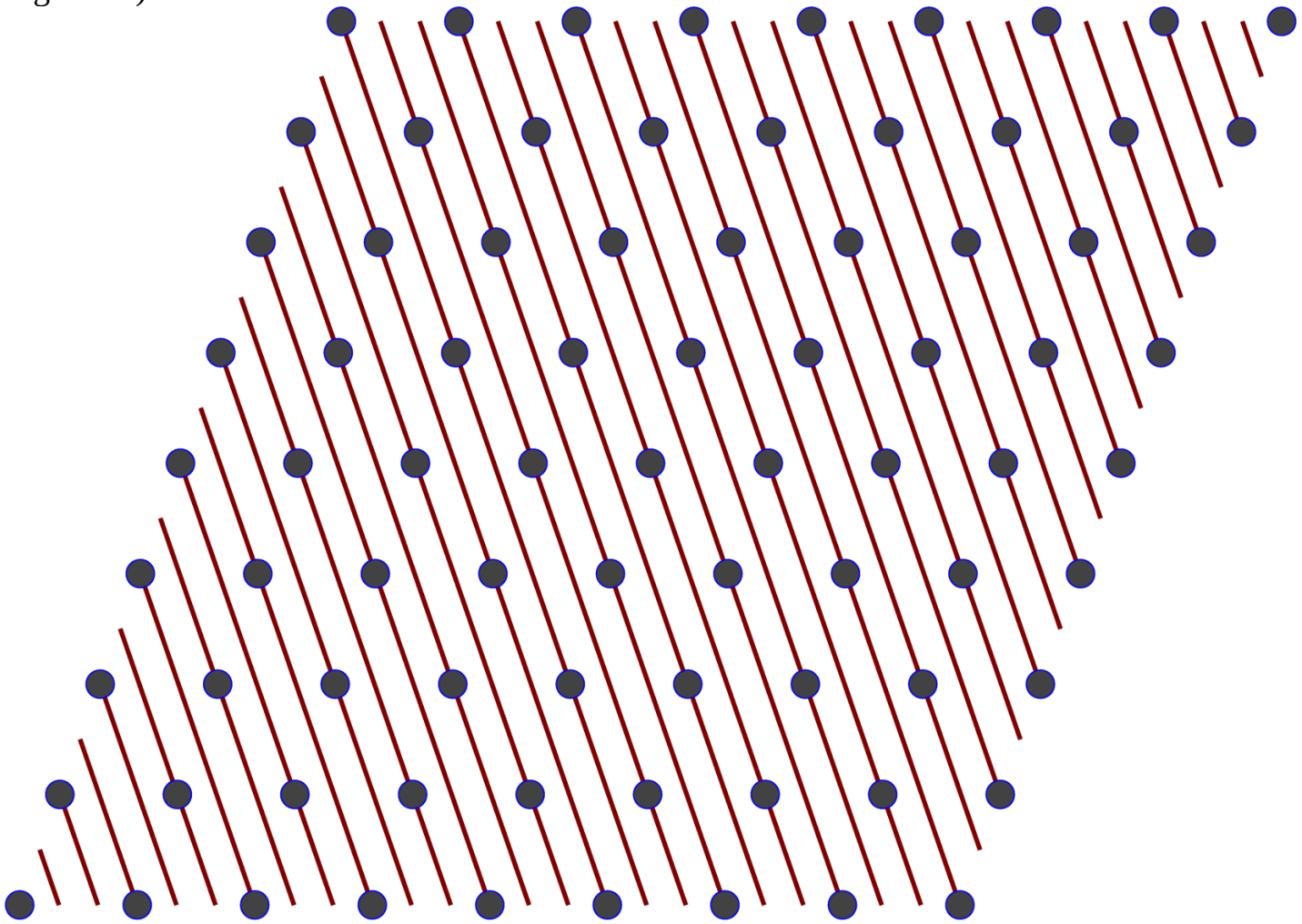
Figure 1a)



UNIVERSITÄT SIEGEN

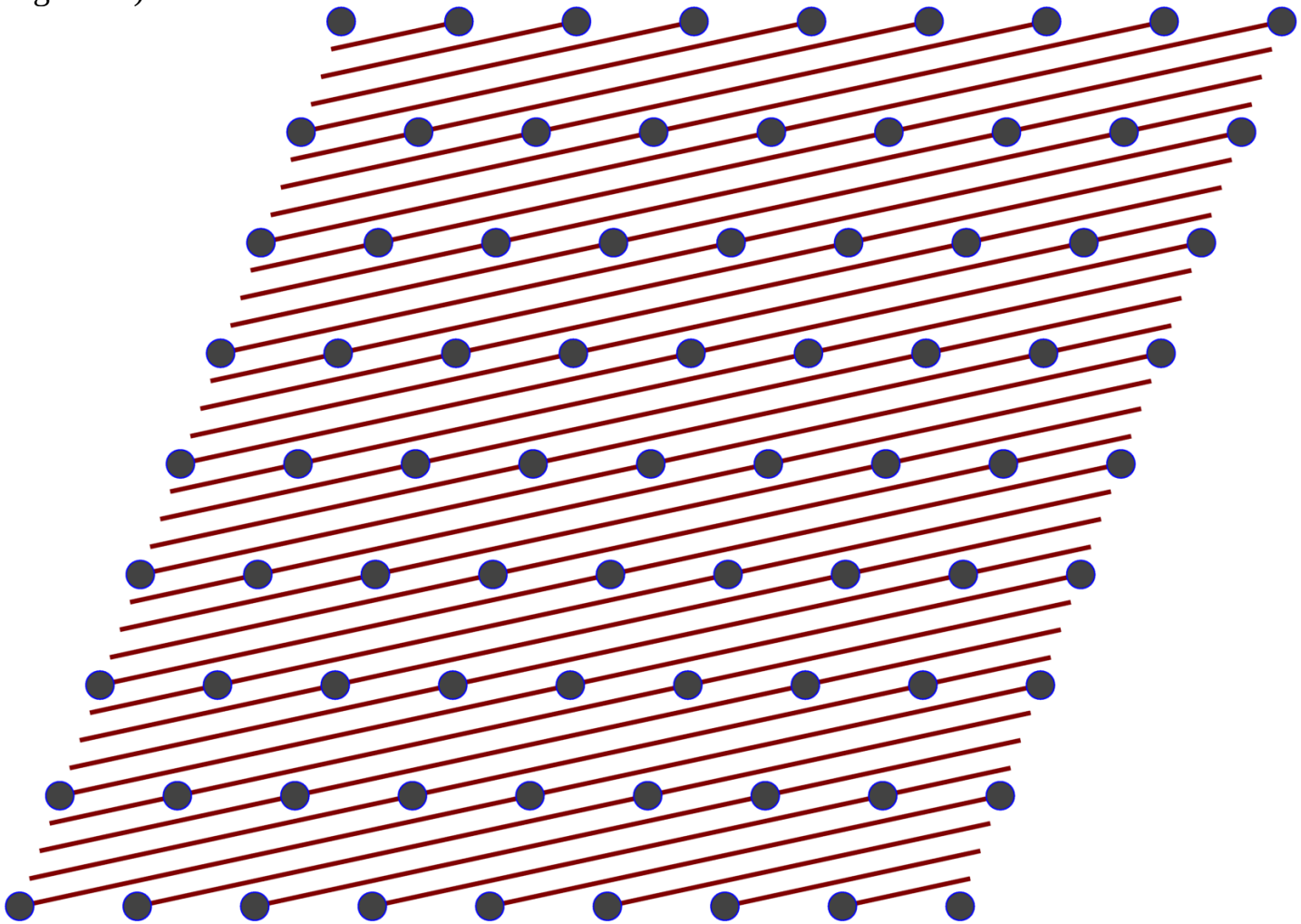
FESTKÖRPERPHYSIK

Figure 1b)



UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Figure 1c)



UNIVERSITÄT SIEGEN
FESTKÖRPERPHYSIK

Figure 1d)