APL 102: Introduction to Materials Science and Engineering – Lab Session

Student Name: Entry No: Lab Group No:

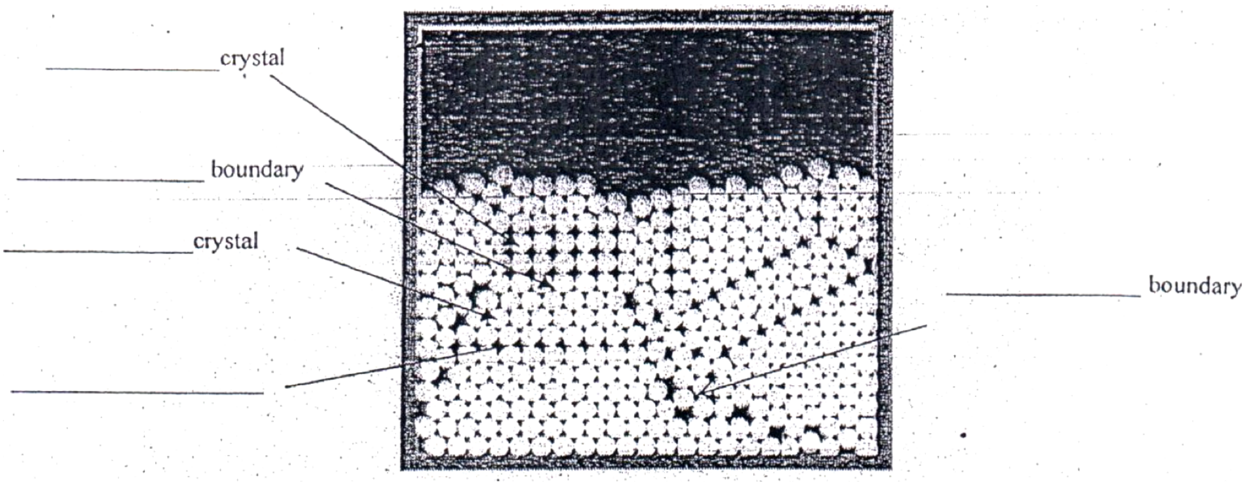
Experiment 7: To study the various models depicting defects in 3D crystalline Structures and 2D graphene

Important instruction:

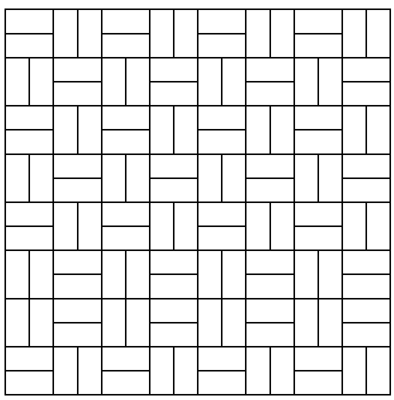
All models used for this experiment are fragile. Do not play with them. You are requested to handle them with extreme care. Do not pull or push on the models while passing it to others.

1. Model 1 (Ball bearing model): Identify the defects in them [2 Marks]

Balls represent hard sphere atoms. By shaking the model you can get the balls in different configurations and see vacancies, grain boundaries, stacking faults and free surface. You can also generate three different phases: square crystals, hexagonal crystal and amorphous phases. By gentle tapping of the model, it is also possible to get the entire model into a single crystal. The following figure depicts one such configuration of balls generated in this model. Here vacancies are not seen but you will find that it gets generated very easily in the actual model. Complete all the labels in the figure giving brief justification.



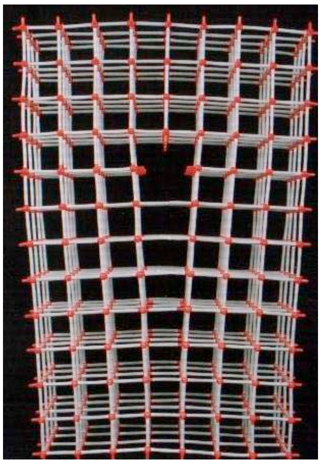
2. Recall that an error was found in drawing of the 99C footpath tiling provided to you Experiment 2 on Two and Three-Dimensional Bravais Lattices. On careful observation it turns out that there is a boundary that separates two otherwise perfect regions of the tiling. Draw this boundary and characterise it, in analogy to defects in 3D crystals, as a dislocation, grain boundary or stacking fault. Give reasons.



3. Model 2 (Edge dislocation): Identify the related characteristics [2 Marks]

You are provided with a model of an edge dislocation, in that:

(a) Locate the extra half plane and the dislocation line by putting a pencil along it.
(b) Select a positive sense of the vector $\vec{t}$ (unit vector tangent to the dislocation line) either going into the model or coming out of it.
(c) Select a starting point and follow a Burgers circuit (Right Hand Finish to Start Rule) around the dislocation. Notice that the circuit fails to close due to the presence of the dislocation. The vector from the finish to start point is the Burgers vector $\vec{b}$ of the dislocation.
(d) Identify the slip plane of the model. The rectangle ABCD, represents the slip plane of the model with AB on the front side. Sketch the dislocation line, the line vector $\vec{t}$ and Burgers vector $\vec{b}$ in the diagram.
(e) Notice that $\vec{t}$ and $\vec{b}$ are perpendicular, a characteristic feature of an edge dislocation.



4. Model 3 (Screw dislocation): Identify the related characteristics [3 Marks]

You are provided with a model of a screw dislocation, in that:

(a) Locate the dislocation line by putting a pencil along it. Note that planes perpendicular to the dislocation line acquire a screw character. Is it a left-kanded (LH) or right-handed (RH) screw dislocation?
(b) Select a positive sense of the line vector $\vec{t}$ (unit vector tangent to the dislocation line) either going into the model or coming out of it.
(c) Select a starting point and follow a Burgers circuit (Right Hand Finish to Start Rule) around the dislocation line. Notice that the circuit fails to close due to the presence of the dislocation. The vector from the finish to start point is the Burgers vector $\vec{b}$ of the dislocation.
(d) A rectangle, representing the slip plane of the model, is shown below. Sketch the dislocation line, the line vector $\vec{t}$ and Burgers vector $\vec{b}$ in that diagram.
(e) Notice that $\vec{t}$ and $\vec{b}$ are parallel (or anti-parallel), a characteristic feature of a screw dislocation.

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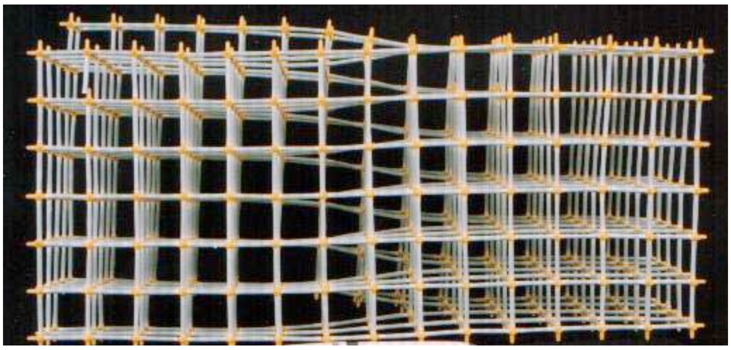


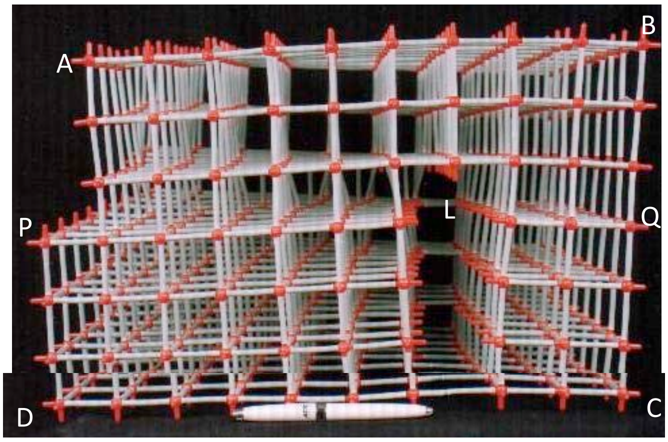
5. Model 4 (Mixed dislocation): Identify the related characteristics [4 Marks]

Two properties of a dislocation:

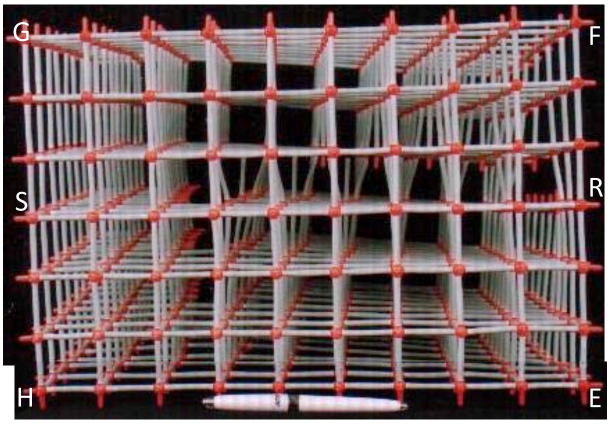
(A) A dislocation cannot end abruptly inside a crystal.

(B) The Burgers vector of a dislocation remains constant.

The front and the back views of this model containing dislocations are shown below:



Front

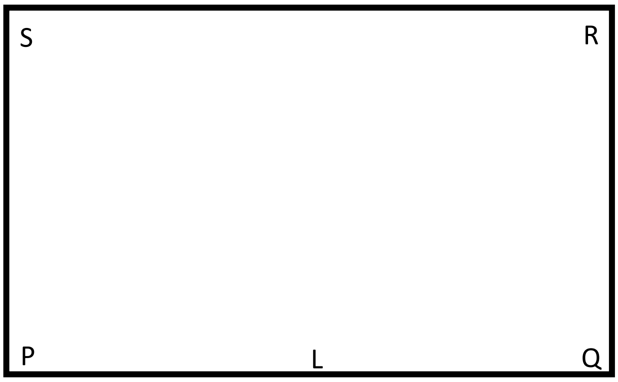


Back

(a) Note that an extra half plane (and hence an edge dislocation) enters into the crystal from the front face at a point marked **L**. However, unlike Model 1, no half plane or dislocation comes out from the back face. Look at the model carefully to resolve this apparent contradiction to the property (A).

(b) Select a starting point and follow a Burgers circuit (Right Hand Finish to Start Rule) around both the end point of the dislocation line and convince yourself that the Burgers vector $\vec{b}$ is the same (property (B)). For this you need to select $\vec{t}$ vectors at the two ends which are consistent with each other, i.e., if it is goes into the model at one end it should come out of it at the other end.

(c) Identify the slip plane of the model. A rectangle, representing the slip plane PQRS of the dislocation in this model, is shown below. Sketch the dislocation line, and choose your line vector $\vec{t}$. Indicate the edge and screw segments of the dislocation line.



6. Other Models: Identify their related characteristics [2 Marks]

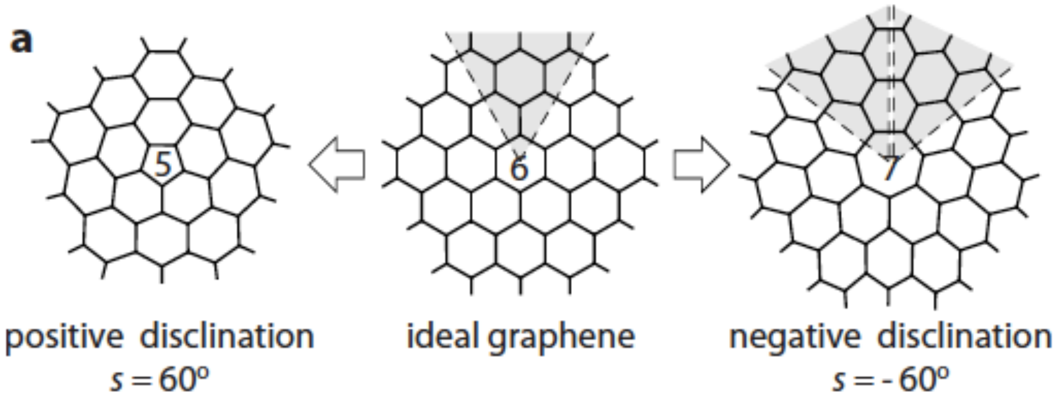
There are other models which you may look at

(a) Prismatic dislocation loops (interstitial and vacancy types).
(b) Tilt and twist boundaries.

Note your observations:

6. Disclinations in Grpahene: [2 marks]

As you have seen, graphene is a two-dimensional crystal with 3-coordinated carbon atoms located at the corners of hexagonal rings. There are two kinds of disclination defects which are possible in the structure. In one case, positive disclination (s=+60º), a hexagonal ring is replaced by a pentagon. In the other case, the negative disclination (s=-60º), the hexagonal ring is replaced by a heptagon. In both the cases the carbon atoms are still 3-coordinated.



[From Oleg V. Yazyev and Steven G. Louie, *Topological defects in graphene: Dislocations and grain boundaries*, PHYSICAL REVIEW B **81**, 195420, 2010]

From one of the patterns of graphene cut out a 60º sector. Although the sector boundary is shown as cutting the bonds perpendicularly, it may be easier to take these boundaries along the C-C bonds. Preserve this sector for the next model. Carefully rejoin the cut edges to create a $+60°$ disclination. Note that flat graphene acquires a curvature. This curvature is like that of a ____________.

From another sheet of hexagonal ring make a cut and insert the 60º sector removed from the previous model. You have now created a $-60°$ disclination. Note that the surface now acquires a curvature. The shape of curvature is that of a ______________.