Homework #3

Miller and Miller-Bravais Indices

Due 5pm Wednesday Oct. 23
Turn in outside of Durand 110 or email to duerloo *at* stanford.edu

1. Structure Determination with HRTEM Images

High resolution transmission electron microscopy (HRTEM) is now capable of showing directly the atomic arrangements in solids, both in perfect and defective crystals. The material is generally aligned with a low index direction (e.g. [100], [110], [111]) parallel to the imaging electron beam whereby the atoms "line up" and are seen in projection. Reference of the image to these low index projections, therefore, allows the study the atomic configurations directly.

The first figure below shows a high resolution image of a FCC Au-Fe nanoparticle with lattice constant 0.39 nm. The scale marker is approximately correct, but not exactly so.

a) Draw several unit cells of the FCC structure projected in the low index orientations [100], [110], and [111]. Compare orientations with the image, and so establish the projection orientation and the viewing direction in the image.
   - One of the crystal viewing web applications mentioned in class may aid in drawing the projections. It may be helpful to eliminate any 3D perspective imposed by the viewer.
   - Note that the spacings of low index (i.e. {100}, {110}, and {111}) planes perpendicular to these three projections differ. If you have trouble establishing the projection plane of this TEM image, you may wish to measure the interplanar spacing of three non-parallel sets of crystal planes in the image using the scale bar and compare with the distances computed for the low index planes visible in the three projections. To maximize the accuracy of your interplane spacing measurements, you may wish to take an average over many planes in the image rather than measure the distance between adjacent planes. Comparison of the angles between low index planes may also help shed light on the projection shown in the image.
   - You could do your measurements using a drawing program (e.g. PowerPoint) or the old fashioned way using a printed version of the image and ruler.

b) Using your knowledge of cubic crystallography, outline the projected FCC unit cell in the drawing. Take the projection to be on either the (100), (110), or (111) plane as you have determined. Now label *consistently* (i.e. not using curly braces for planes) the other low index planes revealed by the HRTEM image using (hkl) Miller indices.

c) In the second figure, an iron nanoparticle is shown. The label of the scale marker has some error: it is closer to 3.6 nm. The nanoparticle could be in either the FCC or BCC structures. From the projections of the FCC and BCC structures onto low-index planes (using a Java viewer or otherwise), determine whether the particle is FCC or BCC and the direction in which it is being viewed. Take the bulk lattice constants for the FCC and BCC Fe to be 0.360 nm and 0.287 nm, respectively. As in part a), indexing the observed crystal planes from their interplanar spacing helps solve the problem.

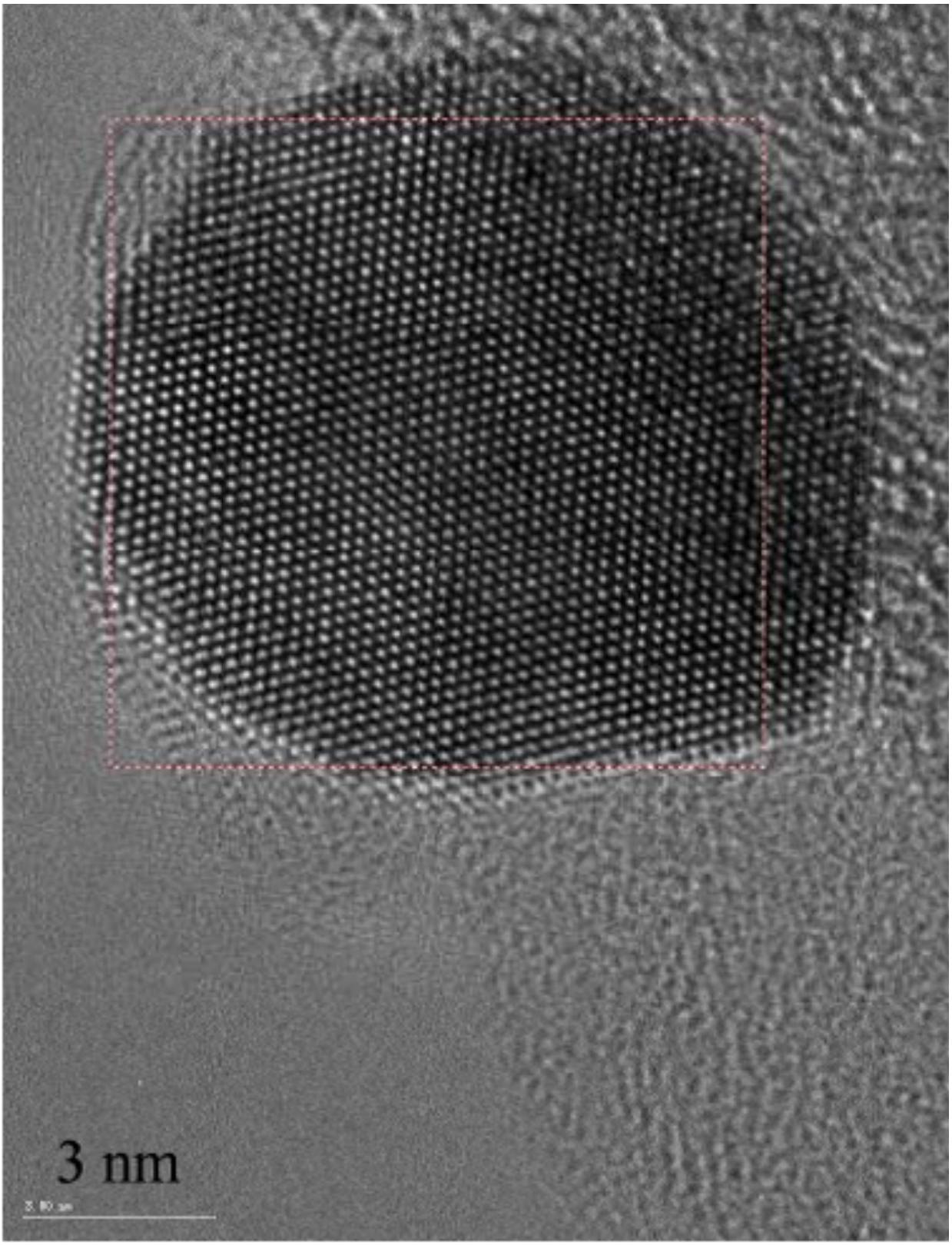

Fig.1: HRTEM of Au-Fe nanoparticle (Courtesy of H. Li, PhD, Stanford University, 2008)

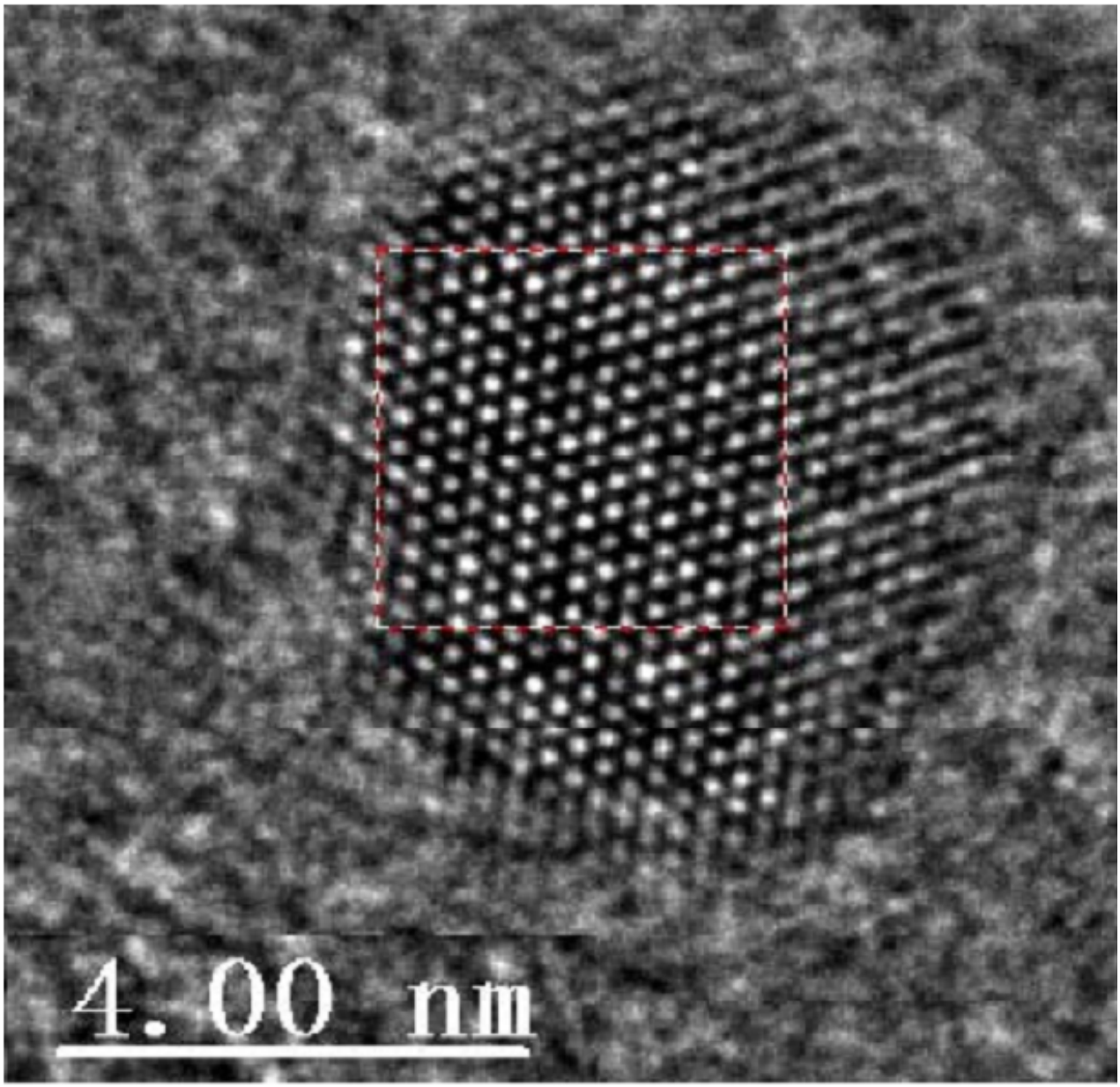

Fig.2: HRTEM of Fe nanoparticle (Courtesy of H. Li, PhD, Stanford University, 2008)

2. Stacking Faults and Miller Indices

Lattice defects play an important role in determining the physical properties of crystalline solids. It is necessary to consider how these defects are introduced into crystals, how they interact with one another, and how they respond to external influences (e.g., shear strains, magnetic fields, etc.). Before this can be attempted, however, we must first understand how their atomic level structure deviates from that of perfect crystals. To this end we will make plane drawings (projections) of the atomic arrangements in several important crystal structures, and then introduce into them several types of lattice defects.

a) Draw to scale the atomic arrangements on the (110) projection of several unit cells of the FCC structure. Across the middle of the drawing, indicate a close-packed plane perpendicular to this (110) section. You may also refer to the schematic on the slide from section 2 titled "FCC intrinsic stacking fault" that shows a (110) projection of FCC.

b) Index *consistently* in the drawing the vertical and horizontal directions in vector notation and the indices of the chosen close-packed plane. Note that the indices of your close-packed plane depend on your choice of vertical and horizontal directions.

c) Identify the length and direction of a Shockley partial dislocation (a/6 $<\bar{1}12>$ displacement vector type), which is parallel to the close packed plane indicated in the drawing. You might consider using the relation from class for the zone axis common to two planes. You can also check your result using the zone law. This vector moves for instance a "**B**" position atom into the "**C**" position. Now, translate ALL the atoms on one side of this plane by this vector, leaving the others stationary. This creates by translation an intrinsic stacking fault. Write down the stacking sequence, and show that it is consistent with an intrinsic stacking fault.

d) Draw the (110) projection of several unit cells of the HCP structure, with the basal planes (close-packed planes) horizontal. Identify the stacking sequence of close-packed planes. As above, establish and give the length and direction (using three-index notation) of a Shockley partial dislocation that lies in the basal plane. Move the atoms in the top half of the crystal with respect to those in the lower half by a translation vector equal to the partial dislocation vector. Determine and write the new stacking sequence.

3. Adventures with Miller and Miller-Bravais Indices

a) Write down the Miller indices (for planes) and zone axis symbols for all possible slip planes and slip directions in fcc and bcc crystals. Slip in these crystals generally occurs on the close or closest-packed plane and in close-packed directions.

b) In an hcp crystal, sketch the (0002) and $\{10\bar{1}1\}$ planes in the $[1\bar{2}10]$ zone. Note the near-hexagonal arrangement of these planes (with angles between planes near 60 degrees) around the zone axis. Determine the value of the ratio of lattice vector lengths c/a for which the arrangement of these planes is precisely hexagonal when viewed along the $[1\bar{2}10]$ direction.

c) Within the $(11\bar{1})$ plane of a face-centered cubic crystal, give all vectors between an atom and its nearest neighbor atoms. You can use the zone law to check that your vectors are parallel to the correct plane.

d) Derive the zone law for Miller-Bravais (4-index) indices using the zone law for Miller (3-index) indices and the transformation relations determined in class.

e) Within the (0001) plane of an hcp crystal, give standard notation 4-index vectors between an atom and all of its six nearest neighbor atoms. Check (or arrive at) your results by permuting the relevant indices.