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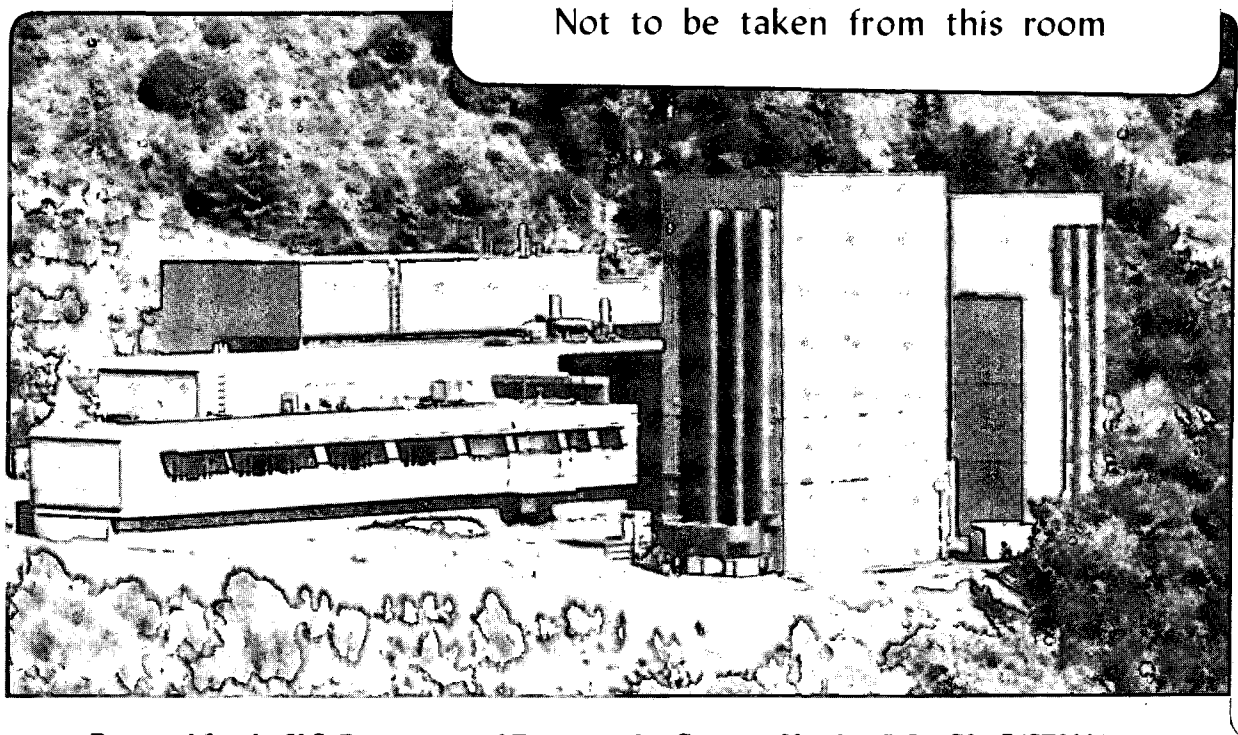

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DEFECT MODELLING IN HRTEM IMAGE SIMULATION

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One practical problem in High Resolution Transmission Electron Microscopy (HRTEM) image simulation is the creation of atomistic models of defect structures. The ideal crystal structures are readily represented by a relatively small number of "basis" atoms and the crystallographic space group. On the other hand, the specification of a grain boundary between two crystals requires the atomic location of possibly thousands of atoms, and a HRTEM simulation program will need all this information before a calculation can be carried out. Users comfortable with writing computer code will write a computer program to generate the hundreds or thousands of atomistic locations, while others may be forced to enter the data by hand or search around for a ready made program that can generate the required data To the authors knowledge, no such suitable program is readily available. There are existing programs that will generate geometric interface models, but these programs were designed to create input to atomistic relaxation calculations, not as generalized tools for creating defect structures.

At the National Center for Electron Microscopy (NCEM) at Lawrence Berkeley Laboratory much work is carried out in the field of image simulation and after spending valuable time writing a one-of-a-kind program each time a new defect structure was to be simulated, it became apparent that a general program was very much needed. A general program for generating interface structures should allow the user to define orientation relationships, specify grain translations with respect to the interface etc., all while graphically displaying the appropriate cross-sections and allowing the user to visually move, delete and add single atoms. Such a program is currently under development at the NCEM and is already changing the nature of how defect structures are created. The input to the program starts with one or two crystalline structures which are either read from structure files created by NCEMSS [1], the image simulation software used at NCEM, or defined by the user by giving the appropriate lattice parameters, the atomic coordinates of the "basis" atoms and the the crystalline space group. In order to create an interface between the two crystals, the user specifies the relationship between the two grains, the interface plane and the zone-axis. The orientation relationship is given either as a pair of parallel planes and parallel directions, or as a common axis and a rotation angle. The interface plane and zone axis are given with respect to either one of the two crystal structures and the program will draw a specified cross section of the resulting interface structure. At this point the user can add translations of the grains with respect to the interface plane, both in the plane and perpendicular to the plane. Atoms that geometrically end up too close to each other can visually be moved around or deleted. Likewise, atoms can be visually added to the structure or substituted by other atom species. By working with a single crystal structure, point defects, voids, etc. can be created. Once the appropriate defect structures are created on the screen a unit cell can be marked by the cursor and by specifying a filename, all relevant information is written to this file, now ready for the simulation calculation. Creating a geometric twin boundary consisting of a few thousand atoms takes only a minute or two. Creating the twin boundary shown in figure 1 took about a minute, and creating a precipitate as shown in figure 2, prior to removing atoms that are too close to each other, took about 2 minutes once the orientation relationship was known. This program is meant to supplement NCEMSS, and like NCEMSS, a public version to run on the Digital Equipment Corporation Vax workstations will be made available as soon as possible.

References

1. Roar Kilaas, Proc. EMSA 45 (1987), 66
2. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

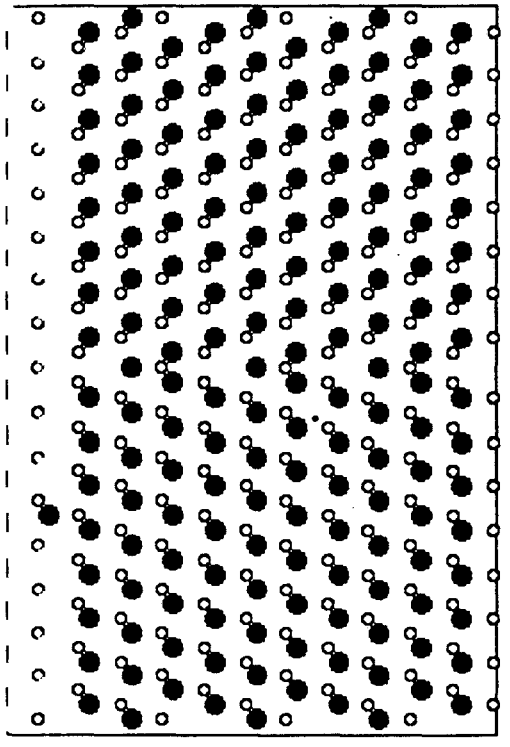

Figure 1.
Twin boundary in Indium Phosphate
Orientation Relationship:
Common Axis: <1,1,1>
Rotation Angle: 180°
Interface plane normal : <1,1,-2>
Zone Axis: <1,-1,0>

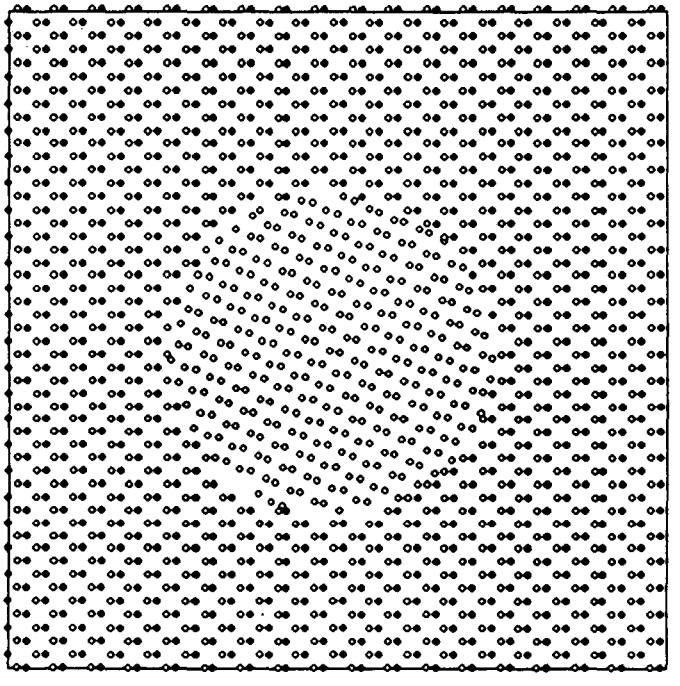

Figure 2.
Precipitate of hexagonal As in a matrix of GaAs.
Orientation Relationship:
$(0,0,1)_{As} \parallel (-1,1,-1)_{GaAs}$
$<0,1,0>_{As} \parallel <0,1,1>_{GaAs}$
Zone Axis: $<0,1,1>_{GaAs}$

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