Simulations of Radiation Defect Images from Transmission Electron Microscopy

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1. Introduction

Defect clusters in irradiated materials occur radiation hardening and embrittlement. Behaviors of radiation defects should be understood to clarify radiation damage mechanisms. Properties of irradiated materials depend on density, size, kinds, microstructure and etc. of radiation defects. These can be measured with transmission electron microscopy (TEM), positron annihilation (PA), small angle neutron scattering (SANS), and 3D atom probe (3DAP). The TEM is undoubtedly the most important technique having made contributions to analysis of characteristics of radiation defects. The TEM is a unique technique, with which a shape and a microstructure of defect clusters can be observed at the images. Radiation defects are mainly dislocation loops. The behavior of a dislocation loop depends on the direction of Burgers vector and a habit plane. Dislocation loops can be observed with a TEM, when the diameter of a loop is larger than 2 nm. When the size is below 5 nm, special cares are required for a determination of directions of the Burgers vector and the habit plane. Generally, **g**•**b**=0 invisibility criterion is used to determine the Burgers vectors of line dislocations. However, when the size is below 5 nm, loops with **g**•**b**=0 are often not invisible and loops with **g**•**b**≠ 0 may also show very weak contrast under weak beam imaging conditions[1]. A special method such as black-white contrast analysis should be used for the determination. This method can be applied to black-white lobe images obtained under dynamical two beam contrast conditions. The directions can be determined roughly with only experimental images. It is needed for a correct determination to match experimental images with computer-generated images. This paper presents results from analyses of dislocation loops with an image simulation technique, TEMACI which was developed by Zhongfu Zhou, the Oxford University.

2. Methods and Results

2.1 Theoretical Basis

The simulation of dislocation loop image was performed with two beam dynamical theory of electron diffraction developed by Howie and Whelan. Though the development of theses simulation programs has been done in 1970s, such program packages can not be available now. Therefore, The Jenkins group of Oxford University developed a simulation program, TEMACI (**TEM** **A**mplitude **C**ontrast **I**maging) which is a computer program for dislocation loop simulation of weak beam diffraction contrasts. When we select two beam dynamical contrast condition at this program, we can get a same effect of images applied with Howie-Whelan equations. Image intensities can be calculated with Howie-Basinski equations as followings.

The wave function of the electron ($\Psi(\mathbf{r})$) can be written as a sum over the diffracted beams $\phi_{\mathbf{g}}(\mathbf{r})$ in the Bloch-wave form[2].

$$\Psi(\mathbf{r}) = \sum_{\mathbf{g}} \phi_{\mathbf{g}}(\mathbf{r}) e^{2\pi i(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})\mathbf{r}} \quad (1)$$

k : the wave vector of electrons incident on the foil.

Sg : the excitation error for the beam with diffraction vector **g.**

The crystal potential is evaluated using the deformable ion approximation.

$$\mathbf{V}(\mathbf{r}) = \sum_{\mathbf{g}} \mathbf{V}_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot(\mathbf{r}-\mathbf{R}(\mathbf{r}))} \quad (2)$$

R(**r**) : the field of atomic displacements around a defect.

By inserting (1) and (2) into the Schrödinger equation and neglecting the second order derivatives, Howie-Basinski equations can be written as following:

$$(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})\cdot\nabla\phi_{\mathbf{g}} = -i\pi U_0\phi_{\mathbf{g}} - i\pi\sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'}) \times U_{\mathbf{g}-\mathbf{g}'} e^{2\pi i(\mathbf{g}'-\mathbf{g})\mathbf{R}(\mathbf{r})} e^{2\pi i(\mathbf{s}_{\mathbf{g}'}-\mathbf{s}_{\mathbf{g}})\mathbf{r}} \phi_{\mathbf{g}'} \quad (3)$$

$U_{\mathbf{g}} = -(2m/h^2)\mathbf{V}_{\mathbf{g}}$, h : the Planck constant

To eliminate the phase factors in Eq. (3), following gauge transformation can be applied.

$$\phi_{\mathbf{g}}(\mathbf{r}) = \Phi_{\mathbf{g}}(\mathbf{r}) e^{-2\pi i \mathbf{g}\cdot\mathbf{R}(\mathbf{r})} e^{-2\pi i \mathbf{s}_{\mathbf{g}}\cdot\mathbf{r}} e^{-i\pi(U_0/(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})_z)\mathbf{r}} \quad (4)$$

The Howie-Basinski equations (3) become

$$(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})\cdot\nabla\Phi_{\mathbf{g}} = 2\pi i(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})\cdot\mathbf{s}_{\mathbf{g}}^{(\mathbf{R})}\Phi_{\mathbf{g}} - \pi i\sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'})U_{\mathbf{g}-\mathbf{g}'}\Phi_{\mathbf{g}'} \quad (5)$$

$S_{\mathbf{g}}^{(\mathbf{R})}$: an effective local deviation parameter that varies spatially when the distortion field $\partial R_i/\partial x_j$ where i, j=1,2, 3.

Eq. (5) can be solved numerically for arbitrarily deformed crystal by dividing it into small cells.

Through consideration of only z direction component of $\nabla\Phi$g, the column approximation can be applied as a following equation.

$$\frac{\partial \Phi_g}{\partial z} = \frac{2\pi i}{\beta_g}(\mathbf{k}+\mathbf{g}+\mathbf{s}_g)\cdot \mathbf{s}_g^{(\mathbf{R})}\Phi_g - \pi i\sum_{g'}(1-\delta_{gg'})\frac{U_{g-g'}}{\beta_g}\Phi_{g'} \quad (6)$$

$\beta_g=(\mathbf{k}+\mathbf{g}+\mathbf{s}_g)$

At Eq. (6), we can get tm of Howie-Whelan equations through considering only two beams of the transmitted and the diffracted.

2.2 TEMACI[3]

The program was written in Fortran 90 format. The program was compiled and run on LINUX systems. It can run under a text mode or a graphic-user interface. The input file is composed with following data:

- Crystal name, job module (1: amplitude images, 2: thickness fringes, 3: multi layer images), column approximation(yes or no), accelerating voltage, defect (edge, screw, loop, void, tetrahedron, 3D-strain or no), image size X-Y, foil thickness, zone axis, beam ranges, (g, ng), anormalous absorption (0: without, 1: with absorption), name of output file, defect nature (perfect, faulted, or pureSF), Burgers vector, stacking fault, size of the loop, position of the loop, loop habit plane, loop plane polar, number of the loop sides and Poisson ratio

2.3 Simulation of two beam dynamical contrast images

With a transmitted beam and a diffracted beam, two beam dynamical contrast images were simulated under a $\mathbf{s}_g$=0 condition. To compare our results with B. L. Eyre et al's[4], a match between our results, we used the same material (Cu), accelerating voltage (100 kV) and foil thickness (1275 nm) loop size (2.4 nm) and with his. Fig. 1(a) is an image under $\mathbf{g}\cdot\mathbf{b}=0$ condition ($\mathbf{b}=1/2\,[01\bar{1}]$, $\mathbf{g}=[200]$). Generally the images of dislocations cannot appear at this condition, because it satisfies the invisibility criterion. But the image of the dislocation loop shows a typical butterfly image. Fig 1(b) shows an image of a Frank loop under a condition of zone axis=$[0\bar{1}\,\bar{1}]$, $\mathbf{b}=1/3[11\bar{1}]$ and $\mathbf{g}=[0\bar{2}2]$. A black lobe and a white lobe are shown evidently.

We could observe changes of loop shape, through changing the position of a loop in a foil.

3. Conclusion

We could set up a computer simulation program of dislocation loop images. We could show that we cannot analyze dislocation loops with only weak beam images of dislocation loops below 5 nm. Through simulations of two beam dynamical contrast images, the ***l***-vector (the direction of Burgers vector) and the ***m***-vector (the direction of habit plane) could be determined. And we could know the shape of dislocation loops changes according to the position into the direction of depth in the foil. Afterwards, we are going to check the effects of loop size, the zone axis, diffraction vector and Burgers vector. This technique can contribute our TEM analysis service for the radiation damage research..

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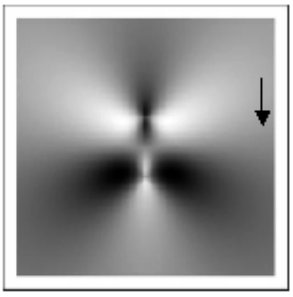
(a)



(b)

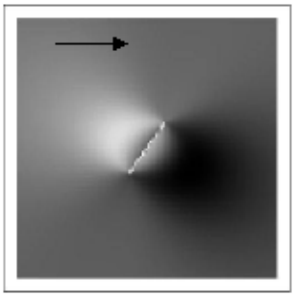


Fig 1. Simulated dark-field images of (a) a perfect dislocation loops with $\mathbf{b}=1/2[01\bar{1}]$, $\mathbf{g}=[200]$ and (b) a Frank loop under two beam dynamical condition and $\mathbf{z}=[0\bar{1}\,\bar{1}]$. The arrow indicates the direction of $\mathbf{g}$.

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