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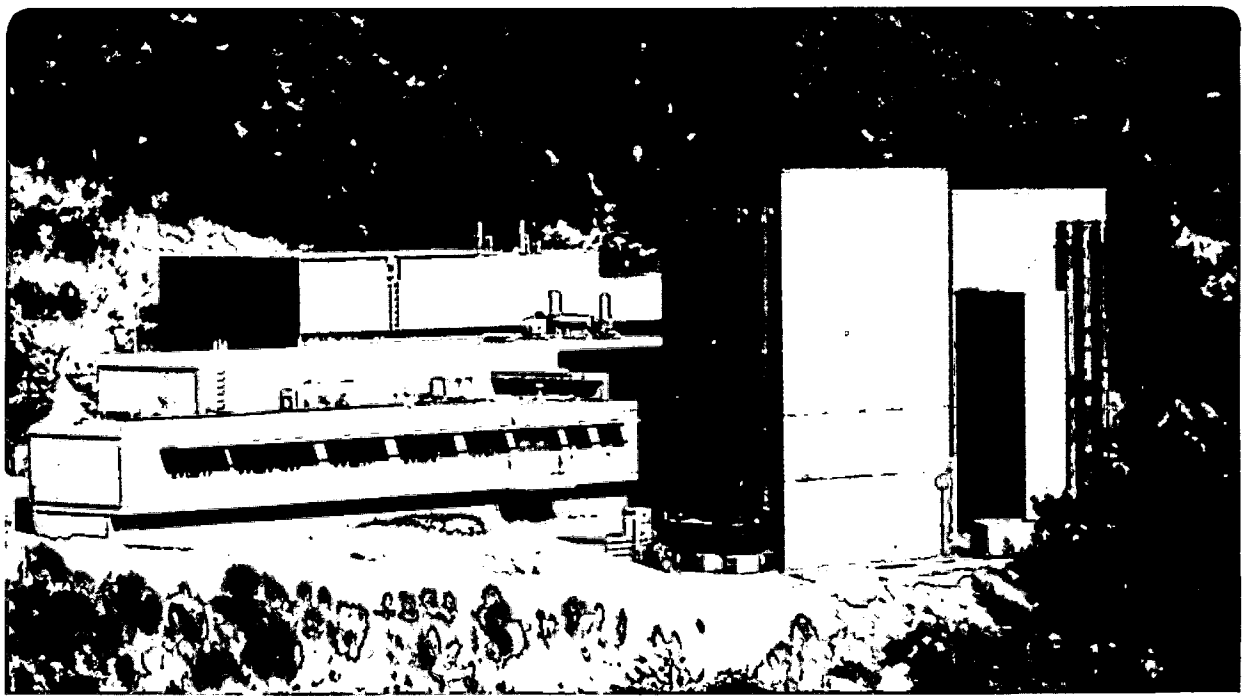

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K.-H. Tsai*, A.F. Schwartzman*, R. Gallego*, M. Ortiz*,
M.A. O'Keefe, & K.-S. Kim*

Materials Science Division
National Center for Electron Microscopy
Lawrence Berkeley Laboratory
University of California, Berkeley, CA 94720

*Brown University
Division of Engineering
Providence, RI 02912

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DETERMINATION OF THE STRAIN FIELD FROM AN HREM IMAGE OF A Si LOMER DISLOCATION

K.-H. Tsai, A.F. Schwartzman, R. Gallego, M. Ortiz, M.A. O'Keefe* and K.-S. Kim

Division of Engineering, Brown University, Providence, RI 02912
*National Center for Electron Microscopy, Materials Sciences Division, Lawrence Berkeley Laboratory, University of California, Berkeley, CA 94720

A novel approach to quantitative deformation characterization of high-resolution electron microscopy (HREM) defect images has been developed. The essential principle of this technique, called Computational Fourier Transform Deformation (CFTD) analysis, is to extract an accurate displacement field about a defect from its HREM image using Fourier transformation procedures. The methodology's unique feature is to digitize the defect image and compute the Moire pattern, from which the displacement field is obtained, without the need for an external reference lattice image, normally associated with the interference phenomena. Details of the image processing steps are described elsewhere.[1] The motivation is that from this data, the displacement gradient can be calculated, which yields much information on the experimental deformation mechanics of some solid undergoing a specific growth process or mechanical testing. One question that has arisen is whether different imaging conditions of the same defect affects the results of the CFTD analysis. We have studied this problem by analyzing the strain components of simulated images of a Lomer dislocation in Si and present our findings here.

The calculation of atom positions about a Lomer dislocation in Si is based on the minimization of the energy of the atomic lattice, employing the Stillinger-Weber interatomic potential.[2] The reason for using this potential is that by careful numerical simulations, Stillinger and Weber demonstrated the ability of their potential to accurately replicate a wide range of physical properties of perfect Si. Image simulations were performed at the National Center for Electron Microscopy at Lawrence Berkeley Laboratory using the NCEMSS computer program. The image simulations are for an 80 Å thick crystal in a JEOL JEM-2010 electron microscope operated at 200 kV and equipped with the ARP pole pieces (a C_S of 1.0 mm, a Gaussian spread of focus of 70 Å, a convergence semi-angle of 0.85 mrad and an objective aperture radius corresponding to 0.6 $Å^{-1}$). The results are shown in Figure 1 for a black atom simulation at Scherzer defocus of -600 Å and a white atom picture at a defocus of -900 Å.

Figure 2 shows the results of the strain components analysis of the simulated images by the CFTD method, along with theoretically calculated images based on anisotropic linear elasticity theory. The dynamic range is ±7%. In previous work, the image processing steps produced a noisy background. The artefact has been suppressed by filtering the whole domain that lies two Burgers vectors away from the core, using a smoothing function that satisfies the equilibrium and compatibility condition for anisotropic linear elasticity. Within the core region, another nonlinear filter is used to remove random noise. We can see excellent agreement for all the strain components, except e_{yy} inside the core region, between the black and white atom image simulations. Thus, the CFTD analysis is insensitive to the imaging conditions of the electron microscope, except for a field of large strain-gradient such as the dislocation core region. For a large strain-gradient field, the HREM image does not represent the lattice configuration accurately. Moreover, the analysis of the simulated images compares well with the theoretical results. In conclusion, the CFTD analysis continues to be a viable procedure for extracting continuum mechanics information from discrete atomic-resolution images of defects in solids.[3]

References

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3. This work was supported by ONR (N00014-90-J-1295) and the Materials Research Group on Micro-Mechanics of Failure-Resistant Materials at Brown University (NSF grant DMR-9002994), and by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under contract no. DE-AC03-76SF00098.

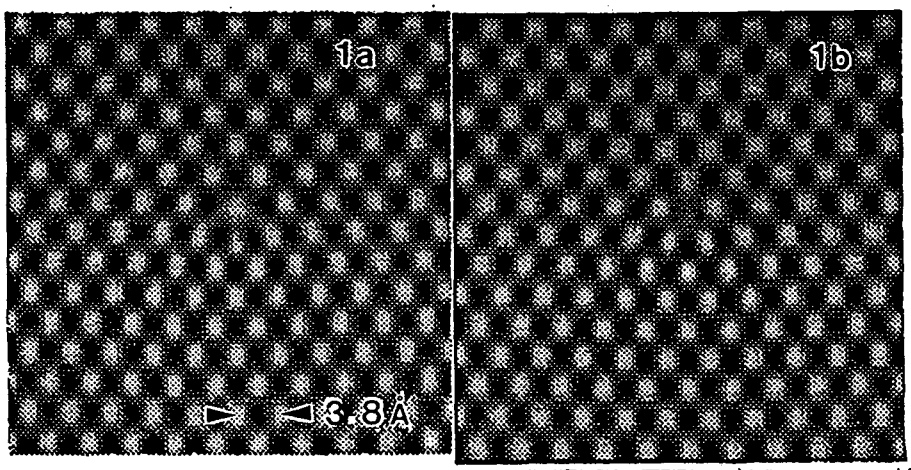
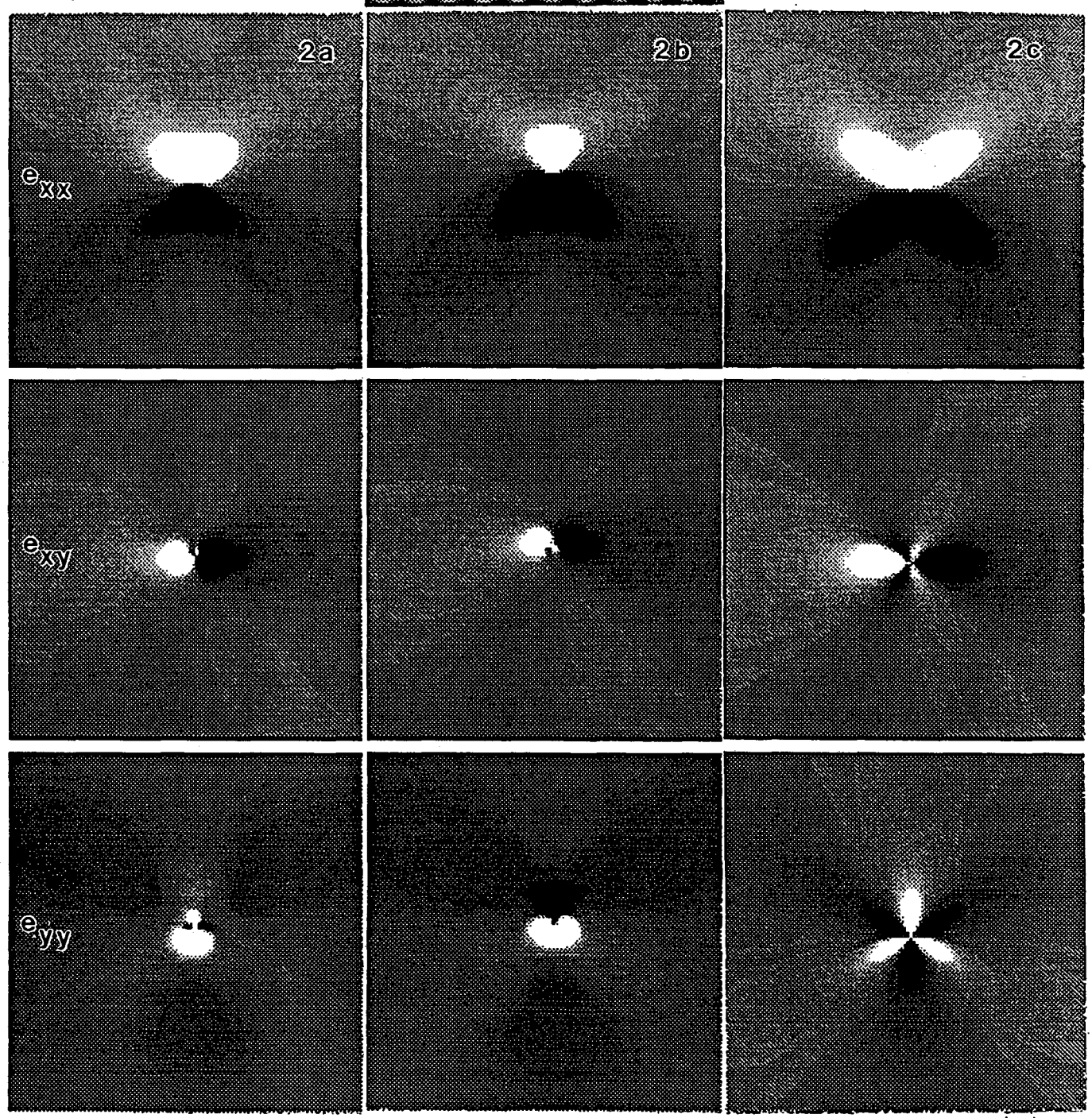


Fig. 1.--(a) Black and (b) white atom image simulations of Lomer dislocation in Si.

Fig. 2.--Strain components analyzed by CFTD method for (a) black and (b) white atom simulations. (c) Theoretical calculations using linear elasticity theory.



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