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Automated Mapping of Lattice Parameters and Lattice Bending Strain Near a SiGe/Si Interface by Using Split HOLZ Lines Patterns

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Accurate measurement of lattice strains in local areas has been growing its importance especially in the modern semiconductor industry because of its strong correlation to the carrier mobility. In the present study, a method to determine lattice parameters and parameters characterizing bending strain of the lattice, the direction and magnitude of the displacement field of the bending strain, by using higher-order Laue-zone (HOLZ) reflection lines observed in convergent-beam electron diffraction (CBED) patterns is proposed. In this method, all of the parameters are determined simultaneously by a fit of two Hough transforms of experimental and kinematically simulated HOLZ lines patterns [1]. This method has been used to obtain two-dimensional maps of lattice parameter *a*, the direction and relative magnitude of the displacement field in a Si substrate near a SiGe/Si interface [2].

Figure 1 shows a schematic drawing of a bent lattice, whose displacement vector **R** varies along the beam direction, *z*. It was found from kinematical simulation that the single major peak of the rocking curve profile with $R_{\max} = 0$ splits into two major peaks whose distance is proportional to $\mathbf{g}\cdot\mathbf{R}$. The linear relation between the split width of the two peaks and $R_{\max}$ was observed for various displacement models. Figures 2(a)-2(c) show HOLZ line patterns simulated by the Howie-Whelan method using different strain parameters. Figures 2(d)-2(f) show HOLZ line positions simulated by the present method superposed by the blue lines. An excellent agreement of the positions of the HOLZ lines indicates the validity of the present method.

A $Si_{0.7}Ge_{0.3}$ crystalline film grown by a molecular beam epitaxy (MBE) technique on a Si substrate was used to test the performance of the present algorithm. The cross sections of the SiGe layers were prepared by mechanical thinning followed by Ar-ion thinning. CBED patterns were taken at an incidence along the [320] orientation from the Si substrate region near the interface, indicated by the rectangle in Fig. 2(a). The probe size of the convergent electron beam was approximately 5 nm in diameter. 10 × 20 CBED patterns were taken from the rectangle area by scanning the probe in *x* and *y* directions with a pitch of 15 nm.

Figures 3(a), 3(b) and 3(c) show maps of the direction of **R**, relative magnitude of $R_{\max}$ and lattice parameter *a* in the rectangle region in Fig. 3(a), respectively. It is clearly visualized that the directions of R are perpendicular to the interface with a slight fluctuation of the direction, and that $R_{\max}$ and *a* show a rather steep increase towards the interface from the area deep in the substrate where the lattice is completely relaxed.

References

[1] K. Saitoh et al., AMTC Letter. 1 (2008) 90.
[2] K. Saitoh et al., submitted to *J. Electron Microsc*. (2010).

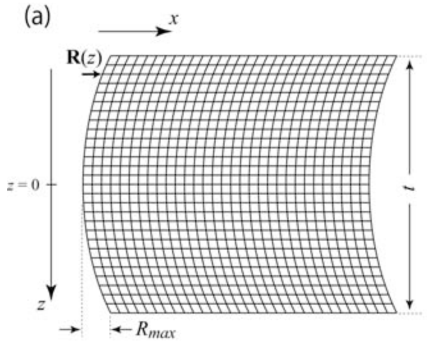

FIG. 1. Schematic diagram of a bent lattice whose displacement varies along the beam direction, z.

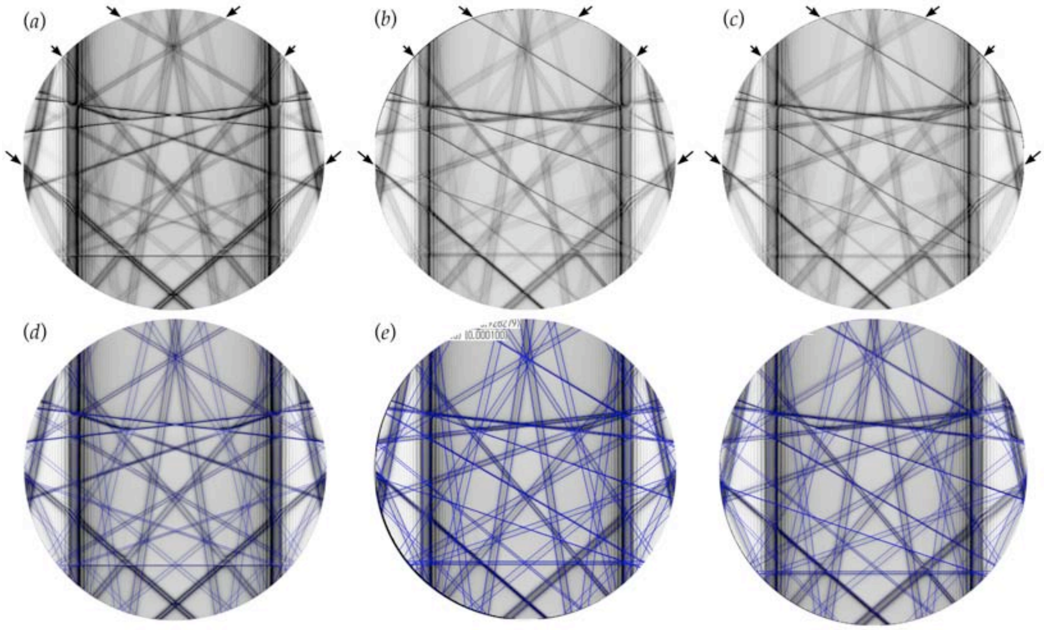

FIG. 2. Si [320] HOLZ line patterns simulated by the Howie-Whelan method and the present kinematical simulation (blue lines) with different bending vectors and lattice parameters. (a), (d): **R** parallel to [001] with R_{max}=1.0, a = 0.543nm. (b), (e) **R** parallel to [239] with R_{max}=1.0, a = 0.543nm. (c), (f) **R** parallel to [239] with R_{max}=1.0, a = 0.550nm.

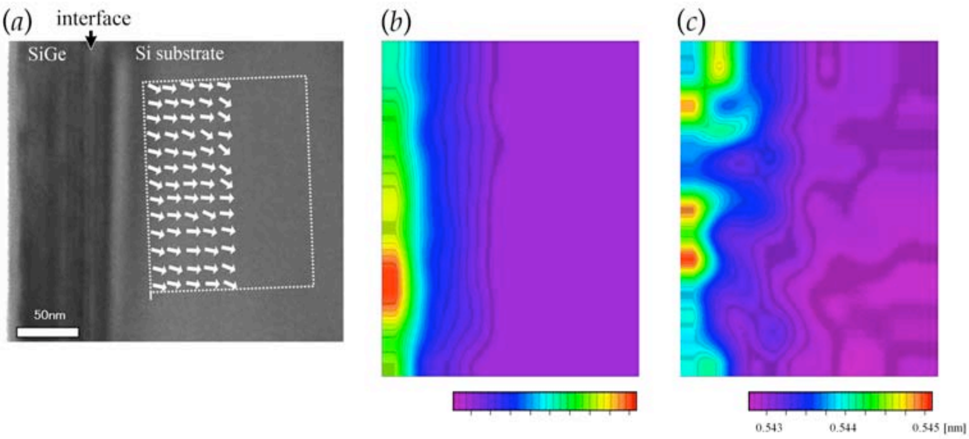

FIG. 3. Maps of the direction (a) and magnitude (b) of bending vector **R** and lattice parameter a (c).