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Dynamic scattering theory for dark-field electron holography of 3D strain fields

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ABSTRACT

Dark-field electron holography maps strain in crystal lattices into reconstructed phases over large fields of view. Here we investigate the details of the lattice strain–reconstructed phase relationship by applying dynamic scattering theory both analytically and numerically. We develop efficient analytic linear projection rules for 3D strain fields, facilitating a straight-forward calculation of reconstructed phases from 3D strained materials. They are used in the following to quantify the influence of various experimental parameters like strain magnitude, specimen thickness, excitation error and surface relaxation.

1. Introduction

Dark-field electron holography (DFEH) is a recently developed technique for measuring strain in nanostructures, in particular over wide fields of view [1,2]. It has been applied to the study of strained-silicon transistors [3–5] and epitaxial thin films [6,7]. Different aspects of the technique itself have been investigated over this period. Precision has been studied as a function of experimental parameters such as exposure time, biprism voltage and sample thickness [8,9]. The methodology has been extended to correct for thickness variations by taking conjugate bright-field electron holograms [2]. The range of imaging conditions, notably magnification and spatial resolution, has been enlarged by adjusting lens configurations [10,11]. However, one particular basic assumption remains unchallenged.

The current assumption when using DFEH is that either (a) the strain is uniform over the thickness of the foil, or that (b) the measured strain corresponds to the average strain over the thickness of the foil. Whilst the former poses no problems within the other assumptions of the method such as the column approximation, such specimens do not exist in practice. Any specimen that had this characteristic in the bulk (indeed, the vast majority of currently studied examples) will have lost it in the process of sample preparation. The two new free surfaces introduced by the thinning process will have relaxed some of the strain through the well-known thin-film effect [12]. More importantly, the strain will now vary over the viewing direction, which we will define throughout as the z-axis. Furthermore, there is a tendency to look at specimens which have z-dependent strain, even in the “bulk”. Two cases in hand are quantum dot structures [8] and modern 3D microelectronic devices such as FinFets [13]. It is therefore vital to know what the measured strain corresponds to exactly.

The problem of z-dependent strain is not new and is inherent to any electron microscopy technique designed to measure strain. The difficulty is always how to evaluate, compensate and correct for it in the analysis. Convergent-beam electron diffraction (CBED), the first technique used to study strained-silicon devices [14], breaks down in the presence of significant column bending due to thin-film relaxation [15]. The only solution is to model the relaxation with an assumed strain field, perform simulations and compare with the experimental data [16]. To avoid brute-force atomistic multislice calculations [17], a Feynman diagram technique applied to dynamic theory was developed [18]. In this approach, the strain is introduced as a perturbation to the full Bloch-wave calculation within the column approximation, and integrated numerically slice by slice through the specimen thickness. A more analytical theory does not currently exist.

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The evaluation of z-dependent strain is perhaps even more difficult for zone-axis techniques such as high-resolution electron microscopy (HRTEM) [3] or nano-beam electron diffraction (NBED) [19]. On one hand, specimens tend to be thinner than for CBED, thus reducing dynamic effects, but on the other hand, the number of beams involved is prodigious. Beyond the woefully inadequate weak-phase object approximation, the only alternative is atomistic multislice simulations, coupled with image formation in the case of HRTEM [20]. Surprisingly, high-angle annular dark-field imaging (HAADF) has seen the most progress towards an analytical approach [21], following on the earlier analysis in terms of strain-induced inter-band scattering [22].

Indeed, we have to return to simpler scattering conditions, such as those prevalent in a DFEH experiment, to find an analytical theory which can incorporate a z-dependent strain field, exemplified by 2-beam dynamical theory [23,24]. Within this theory, analytical solutions were found for some special cases, such as Moiré contrast and stacking fault contrast. These represent a single step in lattice parameter (or strain) or displacement, respectively, within the foil thickness. Other cases have been implemented by a slice by slice approach with transmission matrices (see, e.g., the description in [25]). In the following we will show that the theory can be extended to include a varying z-dependent strain field in a more analytical way.

The organization of the paper follows closely the different levels of approximations used to incorporate strained lattices into scattering theory. After a short introduction to the optical setup of DFEH (Section 2) and high-energy electron scattering (Section 3.1), we discuss the notion of the geometric phase (Section 3.2) as an approximate way to describe weakly deformed lattices. The next step consists of contracting many-beam theory to the experimentally used 2-beam case (Section 3.3). Subsequently, Section 3.4 is devoted to the discussion of special analytic solutions of the 2-beam case. Finally, perturbation theory is applied to analyze the influence of a weakly deformed lattice on scattering under 2-beam conditions (Section 3.5). We use a Si-lattice uniaxially strained along [001]-direction by means of H-ion implantation as model system (see Fig. 1), which is sufficiently simple for our purposes but also technologically important within the so-called Smart Cut™ technology (SOITEC, France). Accordingly, the [004]-diffracted beam has been used for analyzing the strain.

2. Optical setup

To generate a dark field electron interference pattern, a strongly excited diffracted beam is generated by deliberately tilting the specimen into 2-beam conditions. Subsequently, the transmitted beam is blocked by an aperture and diffracted beams originating from an undisturbed and strained specimen region are superimposed with the help of a Möllenstedt biprism to form a hologram in the image plane. This optical setup is illustrated in Fig. 2. The slightly changing diffraction angle within the strained region translates into a

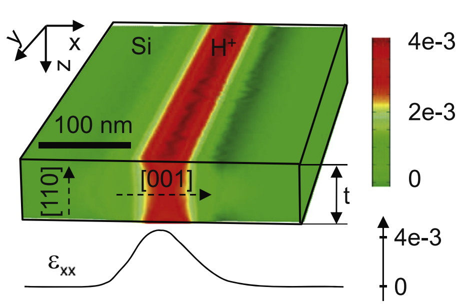

Fig. 1. Strain field $e_{xx}(\mathbf{r})$ generated by H^+-implantation in a Si matrix as calculated by finite element elastic strain theory. Note the significant effect of surface relaxation due to the small TEM specimen thickness and the symmetry of the strain with respect to the middle plane of the specimen. The linescan along x in the middle plane $z=50$ nm approaches the bulk strain of an infinitely thick specimen and will be denoted by e_{xx}^{bulk} in the text.

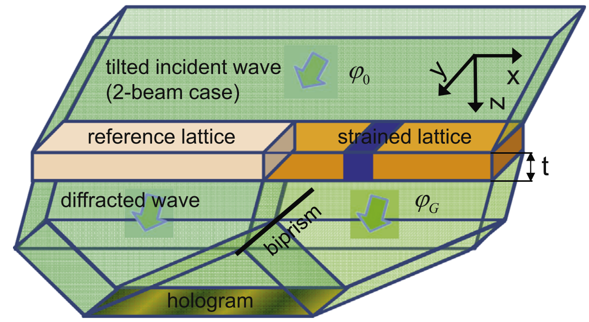

Fig. 2. DFEH setup and coordinate system used in the text. Note that general vectors are denoted by small bold letters, e.g. $\mathbf{r}$, and vectors in $(x, y, z=\text{const.})$-planes will be denoted by capital bold letters, e.g. $\mathbf{R}$.

phase shift in the reconstructed wave which is currently directly interpreted in terms of a z-independent displacement field $\mathbf{u}(\mathbf{R})$, i.e. $\phi_G(\mathbf{R}) = -2\pi\mathbf{G}\cdot\mathbf{u}(\mathbf{R})$ with $\mathbf{G}$ being the reciprocal lattice vector of the diffracted beam [1,26]. From the displacement field one usually derives the components of the physically more significant (infinitesimal) strain tensor $e_{ij} = (\partial u_i/\partial r_j + \partial u_j/\partial r_i)/2$. Additional phase terms are due to thickness variations and misorientation of the sample in combination with dynamic scattering; it has been argued that these phases are small compared to the geometric term [1]. In the following we will refer to reconstructed displacement or strain, when describing the quantity measured by DFEH, in order to distinguish it from the physical displacement or strain of the lattice. Furthermore, we neglect any effect introduced by the aberration of the microscope since modern TEM is equipped with hardware correctors [27], which suppress the influence of aberrations for spatial resolutions in the nm range considered here.

3. Scattering theory

3.1. High-energy electron scattering

We begin our discussion with defining some notation and basic concepts, which will be used throughout the paper: the stationary electron wave function will be denoted by $\psi(x, y, z)$, with z being parallel to the optical axis of the microscope. Planes conjugate to the object exit plane will be described by magnification independent Seidel coordinates [28] $\mathbf{R} = (x, y)^T$. The according reciprocal space coordinates are denoted by $\mathbf{K}$ or $\mathbf{G}$. Consequently, the 2D Fourier decomposition of the wave function reads

$$\psi(\mathbf{R}, z) = e^{i2\pi\mathbf{K}_0\cdot\mathbf{R}} \sum_G \tilde{\psi}(\mathrm{G}, z) e^{i2\pi\mathrm{G}\cdot\mathbf{R}}, \tag{1}$$

where $\mathbf{K}_0 = \sin\boldsymbol{\theta}/\lambda$ is the in-plane component of the electron wave with wave length λ and wave vector $\mathbf{k}_0$ spanning an angle θ with the z-axis. Electrons are scattered by the electrostatic potential $V(\mathbf{R}, z)$ with the according 2D Fourier decomposition

$$V(\mathbf{R}, z) = \sum_{\mathbf{G}} \tilde{V}(\mathbf{G}, z) e^{i2\pi\mathbf{G}\cdot\mathbf{R}}. \tag{2}$$

Furthermore, it is useful to define the so-called interaction constant depending only on the total electron energy E and some fundamental physical constants

$$C_E = \frac{E}{c^2\hbar^2 k_{0z}}. \tag{3}$$

Making use of this notation, the well-known Howie–Whelan (HW) equation, describing the propagation of an electron wave in the small-angle scattering approximation, reads (e.g. [25])

$$\frac{\partial\tilde{\varphi}(\mathbf{G}, z)}{\partial z} = -i2\pi\frac{\mathbf{G}^2 + 2\mathbf{K}_0\cdot\mathbf{G}}{2k_{0z}} + iC_E\tilde{V}(\mathbf{G}, z)\otimes\tilde{\varphi}(\mathbf{G}, z). \tag{4}$$