

Accepted Manuscript

On the Role of the Second-Order Derivative Term in the Calculation of Convergent Beam Diffraction Patterns

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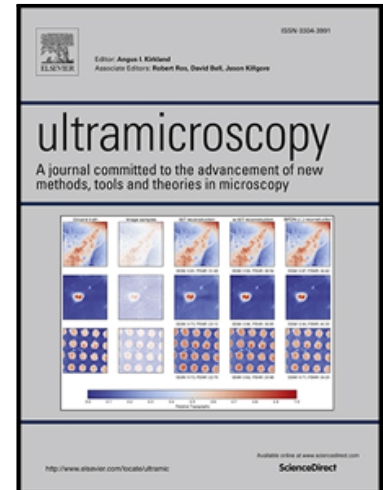
PII: S0304-3991(17)30038-4
DOI: [10.1016/j.ultramic.2017.04.001](https://doi.org/10.1016/j.ultramic.2017.04.001)
Reference: ULTRAM 12348

To appear in: *Ultramicroscopy*

Received date: 21 January 2017
Revised date: 23 March 2017
Accepted date: 4 April 2017

Please cite this article as: S.C. Hillier, E.T. Robertson, G.D. Reid, R.D. Haynes, M.D. Robertson, On the Role of the Second-Order Derivative Term in the Calculation of Convergent Beam Diffraction Patterns, *Ultramicroscopy* (2017), doi: [10.1016/j.ultramic.2017.04.001](https://doi.org/10.1016/j.ultramic.2017.04.001)

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Highlights

- Determined the source of instability in STEM simulations using 2nd-order Schrodinger equation.
- Small amplitude oscillations present in the 2nd-order solution affect numerical efficiency.
- Differences between 1st- and 2nd-order solutions explained using Ewald surface analysis.
- Anti-aliasing of FFTs leads to reduced efficiency of numerical Dormand-Prince 4(5) solver.

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