Time-dependent Eikonal Takagi-Taupin Theory

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Introduction, Methods, and Materials

With the next generation of x-ray sources on the horizon, the ultrafast coherent manipulation and detection of x-rays is becoming an important field of instrumental development. A very promising approach to this task is to induce controlled changes to a crystal, by using a high-power, short-pulse laser. X-ray diffraction from large crystals is described by the dynamical theory of diffraction, and its most successful extensions to deal with statically disturbed crystal are the wave-optical Takagi-Taupin theory and the ray-optical eikonal theory. The two approaches have been synthesized [1-3] into an eikonal Takagi-Taupin theory and have been made explicitly time dependent in a unified space-time approach.

Takagi-Taupin Theory

The dynamical diffraction theory converts the pertinent wave equation into an system of linear equations by use of a Bloch wave, and the derivatives in the wave equation are replaced entirely by wave vectors and frequencies. This yields an algebraic equation that can be solved to obtain the wave (here, electromagnetic) modes inside a crystal (lying on the so-called dispersion surface). The Takagi-Taupin theory [4-6] is an extension of the dynamical diffraction theory to deal with statically disturbed crystals. Recently [1, 2, 7-9], versions of the theory have been developed to address time-dependent disturbances as well.

In the Takagi-Taupin theory, the derivatives of the wave equation are replaced to a large degree by wave vectors and frequencies. However, a fraction of the spatial (and, in the case of the time-dependent theories, also the temporal) variability of the field amplitude is left to be taken up by the remaining spatial (and temporal) derivatives of the field amplitudes. The relative magnitude of this fraction is of the order of the electric susceptibility of the crystal (i.e., typically 10^{-6} to 10^{-5}). Because the disturbance of the crystal cannot be larger than the susceptibility itself, and often is very much smaller, the derivatives of the field amplitudes within the Takagi theory are larger than is necessary to describe only the effect of the disturbance. For the same reason, the Takagi theory lacks the powerful visual language of dispersion surfaces that is developed in the standard dynamical diffraction theory.

As demonstrated by Authier and Balibar, the magnitude of the derivatives can be reduced by a judicious choice of the Bloch base vector [10, 11]. However, this wave vector can not be adapted to the changing conditions that the waves encounter in the course of propagation.

Eikonal Theory

The eikonal theory is a contribution to the overall phase of the Bloch wave that describes the x-ray wavefield inside a crystal. Its gradient and time derivative are contributions to the x-ray wave vectors and frequency. In a perfect crystal, these contributions are constant. When, however, the crystal is disturbed in space or time, then these contributions are generally not constant and reflect momentum transfer and frequency shifts. In the original eikonal dynamical diffraction theory [12-16], it is assumed that the propagation of waves in the crystal can be described in terms of locally approximated perfect crystals, each with its dispersion surface.

Results

Eikonal Takagi-Taupin Theory

When the constant wave vector of the Authier-Balibar theory is made variable, it becomes possible to adapt the wave fields to the variable conditions in a disturbed crystal in such a way that the derivatives of the field amplitudes are minimized. It is, of course, not permissible to change the wave vectors at whim because they must be derived from a phase - the eikonal. Augmenting the Bloch wave of dynamical diffraction with a factor $\exp(i\phi(\mathbf{r},t))$ permits a mathematically correct way of controlling this phase. One may thus vary $\phi(\mathbf{r},t)$ in a numerical procedure to minimize the derivatives of the field amplitudes. These remaining derivatives are ignored in the original eikonal theory. Including them, instead, in a Takagi-Taupin-style differential retains the full wave-optical character of the theory. Because of the minimized derivatives, larger step sizes are possible in numerical simulations, and in some cases, a numerical simulation may become entirely unnecessary because the evolution of the field amplitudes can be read directly from the differential equations [2, 3]. Furthermore, the eikonal equation that minimizes the derivatives gives the best possible approximation to a dispersion surface in a disturbed crystal, making the visual language of standard dynamical diffraction theory available for disturbed crystals, as well. Because the theory is formulated in a unified space-time picture, all of the above applies to temporal, as well as to spatial disturbances of the crystal. The theory can therefore be used as a basis for the design of x-ray optical elements for the subpicosecond coherent control of x-rays.

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References

[1] B. Adams, Proc. SPIE-Int. Soc. Opt. Eng. **4500**, 89 (2002).

[2] B. Adams, in *Nonlinear Optics, Quantum Optics and Ultrafast Pheneomena with X-ray*s, edited by B. Adams (Kluwer Academic Publishers, Boston, MA, 2003), Chap. 3.

[3] B. Adams, Acta Crystallogr. A (in print, 2003).

[4] S. Takagi, Acta Crystallogr. **15**, 1311 (1962).

[5] S. Takagi, J. Phys. Soc. Jpn. **26**, 1239 (1969).

[6] D. Taupin, Bull. Soc. Fr. Mineral Cr. **87**, 469 (1964).

[7] J. Wark and H. He, Laser Part. Beams **12**, 507 (1994).

[8] J. Wark and R. Lee, J. Appl. Crystallogr. **32**, 692 (1999).

[9] P. Sondhauss and J. Wark, Acta Crystallogr. A **59**, 7 (2003).

[10] F. Balibar, Acta Crystallogr. A **25**, 650 (1969).

[11] A. Authier and F. Balibar, Acta Crystallogr. A **26**, 647 (1970).

[12] N. Kato, J. Phys. Soc. Jpn., **18**, 1785 (1963).

[13] N. Kato, J. Phys. Soc. Jpn., **19**, 67 (1964).

[14] N. Kato, J. Phys. Soc. Jpn., **19**, 971 (1964).

[15] U. Bonse, Z. Phys. **177**, 385 (1964).

[16] U. Bonse and W. Graeff, Z. Naturforschung **28a**, 558 (1973).