Dynamic Simulation of a Crystal Lattice under Impulse Loading

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Abstract

A shock front in a crystal is modeled by a displacement of atoms in space and time. The corresponding frequency spectrum is determined via a Fourier transform and represented by 3-D graphics for a range of rise times and types of rise functions. The displacement function has high frequency components which do not depend significantly on the type of rise function.

INTRODUCTION

We are interested in the details of the mechanisms of shock propagation in a crystal. Understanding the details of atomic and molecular positions within the crystal requires the solution of the Schroedinger equation. Understanding the motion of the atoms and molecules within the crystal due to a shock front requires a model for the atomic interaction potential throughout the system. The purpose of this paper is to describe in detail one aspect of a planar shock front, that being the Fourier spectrum of the electromagnetic pulse created by the shock.

ELECTRODYNAMICS OF THE SHOCK FRONT

We consider a shock front incident on a crystal by looking at the displacement of the atoms with time and the related frequency spectrum.

Displacement of the atoms and, consequently, the displacement of the electrons results in moving charge. Radiating, propagating, time-varying fields are the result of accelerating charge. The Lienard-Wiechert potentials (1) describe the radiated electromagnetic fields for a charged particle with arbitrary motion.

The type of time-dependence determines the frequency of the radiation. Sinusoidal time variation has one frequency (e.g. simple-harmonic oscillator). A non-harmonic time dependence will have more than one frequency with the exception of a constant with respect to time, which has no frequency (d.c. component). The Fourier transform of a time-domain function gives the corresponding frequency spectrum.

We consider a planar displacement of the atoms in the crystal as shown in Fig. 1. The shock front initially displaces the first plane of atoms by a certain distance. The plane of atoms then moves back to its original position. This is a simplified

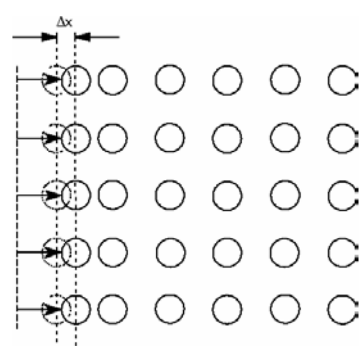

FIGURE 1. Planar displacement of atoms due to a shock front impulse.

model to obtain some initial results; the actual displacement of the atoms is more complex than what we have considered here.

We represent this planar displacement by a function dependent on time as shown in Fig. 2. This is essentially a superposition of a rect function with a rise time function and a fall time function. A rect function is defined as a constant amplitude value from one point in time to another point in time and is zero elsewhere. The rise/fall times are on the order of 10-100 femtoseconds. Note that the rise and fall times are defined as time for displacement from 10% to 90% of peak value. The

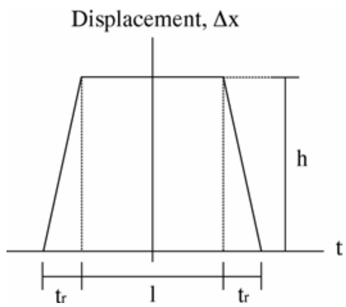

FIGURE 2. Representation of the planar displacement with respect to time.

rect function has a length of 1 picosecond, which is the time between initial displacement and return displacement. The maximum displacement is defined to be 10^{-12}; however, any value of height will suffice, as it is only an amplitude scale factor.

Four types of rise/fall functions are used: ramp, cosine, Gaussian, and Fermi functions. The constants for each of these functions are dictated by the choice of the rise time. See Figs. 3-6 for an example of each of the four representations of the displacement.

The Fourier transform is determined for each type of displacement by using the computer package Mathematica®. The Mathematica® command to obtain the frequency spectrum for the displacements with ramp and Gaussian rise functions is: G(ω) = FourierTransform[g(t), t, ω]. This corresponds to the definition of Fourier transform:

$$G(\omega) = \int_{-\infty}^{\infty} g(t) e^{-j\omega t} dt \qquad (1)$$

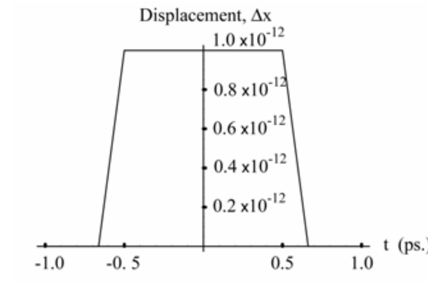

FIGURE 3. Displacement with ramp rise function, t_r=100 fs.

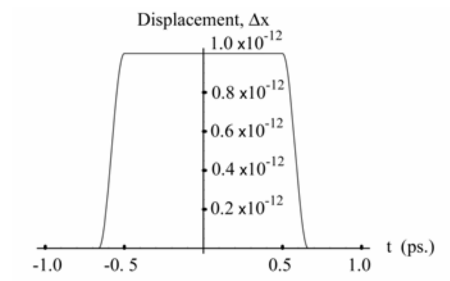

FIGURE 4. Displacement with cosine rise function, t_r=100 fs.

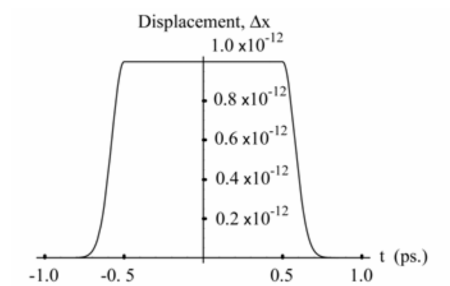

FIGURE 5. Displacement with Gaussian rise function, t_r=100 fs.

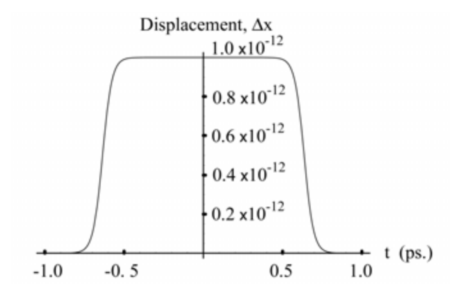

FIGURE 6. Displacement with Fermi rise function, t_r=100 fs.

where g(t) is the time-domain function to transform, t is the time variable, ω is the angular frequency variable, and G(ω) is the frequency-domain variable.

The Fourier transforms for the cosine and Fermi functions are not directly determined by the "FourierTransform" command. A numerical calculation using "NIntegrate" (2), a Mathematica® command for numerical integration, along with the definition of Fourier transform in Eqn. 1 is necessaryWe compare the frequency domain results for different rise times by using 3-dimensional graphics for each displacement type to show the variation in the spectra for a range of rise times. We also want to compare the results between the four cases. We graphically display the data using "ListPlot3D" (2), the Mathematica® command for 3-D graphics for numerical data. The resulting 3-D plot represents the frequency spectra for a range of rise times. The plots for the cases of the ramp, cosine, Gaussian, and Fermi rise functions are Figs. 7, 8, 9, and 10 respectively.

The rise times for these plots range from 10 fs to 100 fs. A wider range of rise times could have been shown, but these values are sufficient to depict the characteristic trends as rise time changes. The amplitude on the plots is the log of the normalized displacement function. The displacement function, Δx_N (ω), is normalized by dividing by one unit of the chosen displacement units.

These displacement time functions are essentially rect functions with the rise times two orders of magnitude smaller than the time duration between rise and fall. So, it is not surprising that

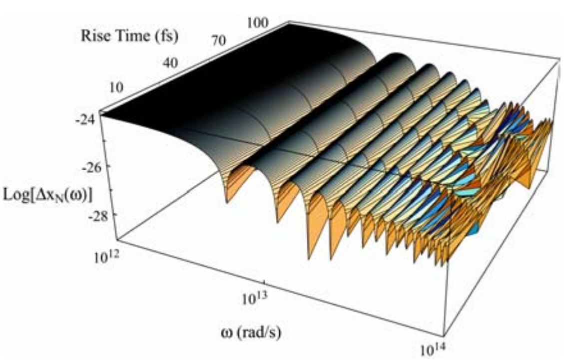

FIGURE 7. Frequency spectra of the displacement with ramp rise function with range of rise times from t_r=10-00 fs.

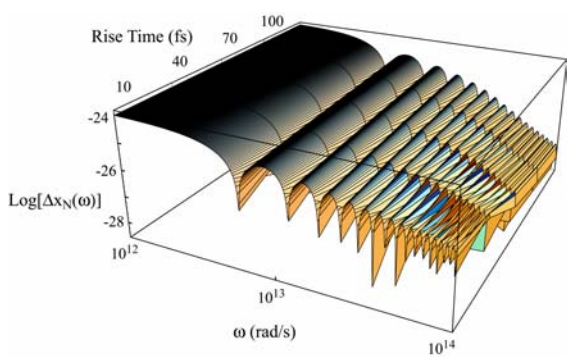

FIGURE 9. Frequency spectra of the displacement with Gaussian rise function with range of rise times from t_r=10-00 fs.

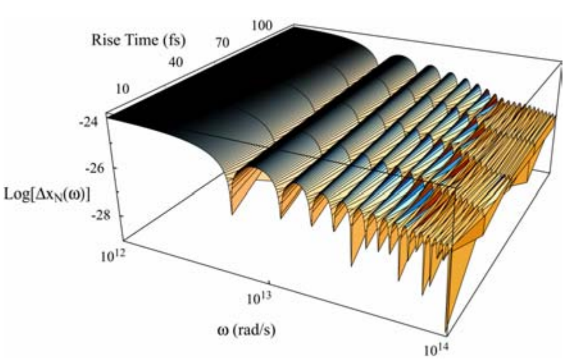

FIGURE 8. Frequency spectra of the displacement with cosine rise function with range of rise times from t_r=10-00 fs.

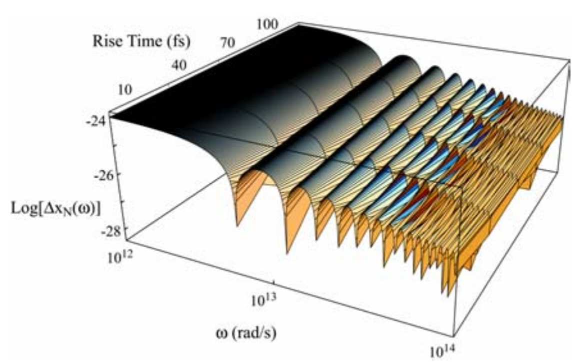

FIGURE 10. Frequency spectra of the displacement with Fermi rise function with range of rise times from t_r=10-00 fs.

the resulting frequency spectrum is very similar to a sinc function. A sinc(z) is defined as the ratio: $\sin(\pi z)/(\pi z)$. A rect function with a total length of 10^{-12}s transforms to a sinc frequency function with its first null at an angular frequency of $2\pi x10^{12}$ rad/s. The frequency plots show that the first null is approximately in the range of $2\pi x10^{12}$ rad/s. Of course, the actual displacement function used is not a perfect rect function. Therefore, while the resulting frequency plots are not perfect sinc functions, they are very similar.

An impulse function (i.e. Dirac delta function, a spike with infinite amplitude at one point in time) transforms to a constant value for all frequencies. The displacement time functions are similar to impulses in that they have a very short time span. If the displacement amplitude is large enough, then we could consider this an impulse, which would result in a constant value for all frequencies. Of course, this is not true as seen from Figs. 7-10; however, we do see that amplitude is approximately constant out to angular frequencies on the order of 10^{12} rad/s.

The frequencies spread out as the rise time decreases. In other words, the position of a null increases in frequency as the rise time decreases. Correspondingly, the amplitude of the frequency spectrum decreases as the frequencies spread out. Because the rise time is not changing drastically in magnitude, the change in amplitude and in positions of the nulls is quite small.

Minor peaks are present in the frequency spectra for the ramp rise function displacement (Fig. 7). These are present because of the sharp transition from the rise function to the rect section of the displacement. Convolution of two rect functions of different lengths in the time-domain results in a rect funtion with ramp rise functions and is equivalent to multiplication in the frequency-domain of two sinc functions having different null positions and amplitude fall-off rates. The sinc function arising from the shorter rect function will bound the sinc function arising from the longer rect function, which results in a form of "amplitude modulation" corresponding to the additional peaks seen in Fig. 7.

What happens to the spectra at even higher frequencies? The trend is similar. Consider the rect rise function case plotted out to 10^{20} rad/s as seen in Fig. 11. The amplitude still decreases as frequency increases, and the same spreading out of the nulls in frequency occurs, as with the plot showing the lower frequencies (Fig.7).

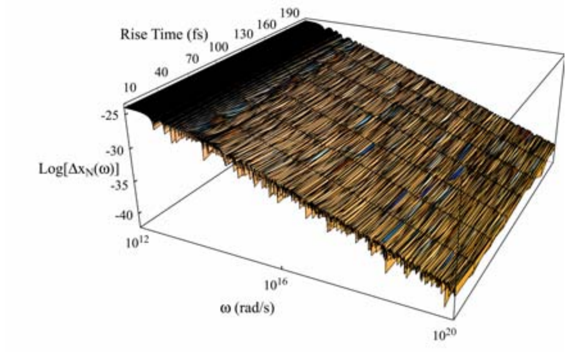

FIGURE 11. Frequency spectra of the displacement with ramp rise function with range of rise times from t_r=10-190 fs.

CONCLUSIONS

Examination of the results for the planar displacement of the atoms brings forth several generalizations. The frequency spectrum has appreciable amplitude out to high frequencies. The frequency spectrum does not depend significantly on the variation of the type of rise function impulse as seen in the comparison of the four displacement functions. If the shock front impulse is similar to this form, the high range of frequencies with substantial amplitude will be present. Further research in this area is necessary to provide a link between the results presented here and the physics of shock propagation in condensed matter.

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