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Prediction of coherent optical photons from shock waves in crystals

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In this work, we study the electromagnetic radiation emitted by the propagation of a shock wave through an ionic crystal, NaCl. Our analytical theory and computational experiments predict that under some conditions, weak yet measurable temporally coherent light can be observed emerging from the crystal, typically in the range 1-100 THz. [1] The radiation is generated by an oscillating dipole-like material polarization resulting from the nonlinear synchronized motion of large numbers of atoms induced by a planar shock wave propagating through the crystalline lattice. To our knowledge, coherent emission in this frequency regime has not been observed from a shocked crystal because it is in a portion of the electromagnetic spectrum that is usually not observed in such experiments and some experimental care must be taken to realize the appropriate conditions under which the effect can be observed.

As a shock propagates through a polarizable crystal, a change in polarization can be induced which yields a time-dependent polarization current (even in materials with no static polarization). [2, 3] While it is not surprising that radiation should be emitted from polarization currents induced by the shock (e.g., thermal emission), it is unexpected that this emission should be of a coherent nature. In this work, we consider a special case of shock-induced polarization that occurs only in crystalline materials when the shock front becomes very sharp, i.e. the shock rise distance is a few lattice planes of the crystal or less. Figure 1 shows a schematic depicting a fashion in which a temporally-periodic polarization can arise in a shocked polarizable crystal as a result of athermal motion of the atoms. Red and blue atoms on the left represent positively and negatively charged atoms. Atom positions within the shocked crystal are shown at four instances in time on the left with a gray area highlighting the shock front region. As the shock propagates over each lattice plane (left to right) the symmetry of atoms in that lattice plane can be temporarily broken yielding a non-zero static polarization of the atoms at the shock front. In Figure 1, the static polarization points perpendicular to the plane of the shock wave. The broken symmetry can result from the atoms being different types with different masses or it can have other origins. The transient static polarization produced each time the shock propagates through a lattice plane of the crystal yields a temporally periodic polarization current which can potentially emit coherent radiation.

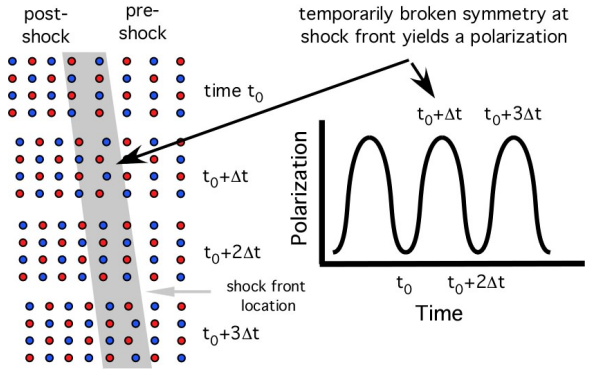

FIG. 1: Schematic depicting a fashion in which a temporally-periodic polarization can arise in a shocked polarizable crystal. As the shock propagates over each lattice plane (left to right) the symmetry of atoms in that lattice plane can be temporarily broken yielding a non-zero static polarization of the atoms at the shock front. See text for details.

Using a Bloch-like symmetry analysis of this system, we show that possible frequencies of the generated polarization currents are, $\omega \approx 2\pi\ell\frac{v_s}{a}$ where v_s is the shock speed, a is the crystal lattice constant and ℓ is an integer. The frequencies of the polarization current are associated with the temporal period of the shock propagating through a single lattice unit of the crystal.

We have numerically explored this effect using using an analytical approach, finite-difference simulations of Maxwell's equations, and molecular dynamics simulations. In what follows, we focus on molecular dynamics simulations of shock waves propagating through crystalline NaCl. Such commonly utilized simulations solve the classical equations of motion for atoms subject to an empirically-constructed interaction potential and incorporate thermal effects and deformation of the crystal lattice. In these calculations, planar shock waves are generated within 3D computational cells of perfectly crystalline atoms at T=4.2K by constraining atoms at one edge of the long dimension of the computational cell to move into the cell like a piston (representing the mechanical driving force or object that generates the shock). An infinitely planar shock propagates away from the constrained atoms into the the computational cell. The shock propagation direction component of the total electric polarization current is $J = \sum_i v_{z,i} q_i$ where q_i is the charge and $v_{z,i}$ is the shock direction (z) component of

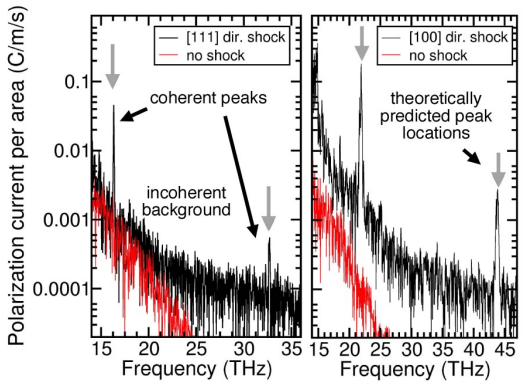

FIG. 2: Fourier transform of the electric polarization surface current component in the shock propagation direction for molecular dynamics simulations of a shock propagating through NaCl in the [111] direction (left) and [100] direction (right). Narrow bandwidth, coherent peaks exist in the shocked simulations (black) that do not exist in the simulations without shocks. Thermal noise gives rise to an incoherent background.

the velocity of atom i.

Figure 2 shows results of about 30 ps duration simulations of shocks propagating in the [111] and [100] directions initiated with piston velocities of 200 m/s. This relatively small piston velocity generates a shock that applies a uniaxial strain of 0.03-0.04 to the post-shock material and increases the material temperature less than 1K. Figure 2 compares the shocked and unshocked Fourier transform of the shock propagation direction component of the total electric polarization current in the computational cell. Narrow peaks are observed in the shocked simulation that do not exist in the unshocked simulation. From the peak widths, the coherence length of the radiation emitted in vacuum is determined to be about 5mm and 3mm for the 16 THz, [111] peak and 22 THz, [100] peak, respectively.

The relation $\omega \approx 2\pi\ell\frac{v_s}{a}$ predicts that emission should occur in multiples of 5.4 THz in the [111] case since the periodic unit for the [111] direction in NaCl $a = 9.78$Å and the shock speed observed in the simulation is $v_s = 5300m/s$. The 16 THz and 32 THz peaks on the left of Figure 2 correspond to 3 and 6 times the fundamental frequency of 5.4 THz ($\ell = 3$ and $\ell = 6$,) in excellent agreement with theory (gray arrows). The 16 THz peak can be attributed to structure within the unit cell of distance $a = 3.26$Å (i.e. $\ell = 1$ if $a = 3.26$) which is the distance between atomic lattice planes of like charge in the [111] direction (the NaCl crystal consists of alternating planes of positively and negatively charged atoms in the [111] direction.) A similar analysis applies to the [100] shock direction case.

The radiation distribution properties can be calculated using the polarization current amplitudes from the planar shocks of the molecular dynamics simulations. A particularly simple case is when the shock front diameter is much less than the wavelength of the coherently emitted radiation. In this case, the shock wave acts as an oscillating dipole. For a $5\mu m$ diameter shock front in the case of the 22 THz peak on the right side of Figure 2, 3×10^{11} Watts are radiated while the shock propagates. Collected and focused, this radiation yields an electric field amplitude up to about 0.1 V/cm. The field strength and radiated power are sensitive to the curvature, roughness, and area of the shock front and can potentially be increased by orders of magnitude in other scenarios. The energy conversion efficiency for generation of this radiation is likely to be extremely small since far more energy is required to physically compress the material than to produce the radiation.

The 16 THz and 22 THz peaks in Figure 2 have frequencies that are up to two times higher than phonon frequencies; the peak frequencies are not associated with any phonon frequencies. Observation of these peaks requires that there be spectral components of atom velocities at these higher frequencies around the shock front. Such high frequency components of atomic motion can be generated only if the shock front (or part of it) is very sharp.

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