Ultrafast Cellular Automata Dynamics of Phase-change Optical Response

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We introduce a cellular automata methodology for studying photonics of light-induced phase transitions. Multiphysical complexity over disparate length/timescales is reduced to a simple, heuristic rule/parameter set in a model successfully describing several independent experimental datasets.

Phase-change Photonics
- Light-induced structural transitions are of enormous technological importance and fundamental scientific interest.
  - optical data storage
  - controlling laser dynamics
  - optical and plasmonic modulation
- Light-induced structural transitions are of enormous technological importance and fundamental scientific interest.
- ... BUT comprehensive modelling is extremely challenging, involving
  - atomic/molecular structural change
  - inhomogeneous change of optical properties
  - time & length scales spanning many orders of magnitude
- A cellular automata (CA) model can capture this complexity in a sparse set of ‘evolutionary’ rules

CA Model for Gallium Phase-change Nonlinearity
- Solid Ga near its bulk melting point (Tm = 29.8°C) manifests a gigantic, broadband phase-change nonlinearity underpinned by thermal + non-thermal light-induced surface metallization.
- CA model for metallization dynamics: 2D array of Ga (crystalline unit) cells; 3 states; 4 transition rules applicable in each time step.

Femtosecond Optical Excitation
- Pump pulse at incident on planar silica/Ga interface, Δν = 773 nm, 3 mJ/cm², τp = 1 fs; τs = 1 ns
- Corresponding sharp reflectivity increase.

Dynamics & Microscopic Mechanism vs. Pulse Duration
- Short pulses (τs < τp): Diffuse EXCITED/METALLIC cell population in GROUND state Ga bulk; No change in surface-melt layer thickness at interface. Two-step reflectivity increase - initially sharp then slower rise.
- Long pulse regime (τs >> τp): Growth of METALLIC surface-melt layer into Ga bulk. Proportionate, steady increase in reflectivity during pulse.

Recrystallization
- CA reproduces experimental pump-probe measurements of fs-ps Ga/silica interface reflectivity dynamics, supporting prior inference of diffuse ‘fractional melting’ mechanism.

Summary
- Cellular automata successfully describe, non-stationary, spatially inhomogeneous dynamics and resulting nonlinear optical properties of a medium undergoing a light-induced structural transition.
- Minimal CA transition rule and physical parameter set reproduces experimentally observed behaviours over seven orders of excitation pulse duration (fs-ps), providing insight to microscopic mechanisms.
- CA methodology easily adaptable to different physical systems and nano- to macroscopic sample structures.


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