Phase-change Optical Nonlinearity as a Cellular Automaton

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We introduce a cellular automata methodology for studying photonics of light-induced phase transitions. Such transitions underpin some of the most important emerging 'reconfigurable' photonic technologies but are a complex tangle of processes developing simultaneously over length and time scales spanning several orders of magnitude: atomic/molecular structural change, band-structure modification, domain/crystallization dynamics, inhomogeneous change of optical properties, and heat/light transport/dissipation. As such they present significant challenges to both theoretical and numerical modelling approaches. Here, we show for the first time that the problem of describing such complex nonlinear optical processes in phase change materials can be reduced to one of just a few free parameters and evolutionary rules in a classic cellular automata (CA) model.

We consider solid gallium near to its bulk melting transition, as a non-trivial system in which optical excitation may proceed via both thermal and non-thermal mechanisms, and surfaces are subject to nanoscale 'pre-melting'. This CA model reproduces experimentally observed light-induced transition and relaxation dynamics of gallium over seven orders of excitation pulse duration magnitude from femtosecond to microsecond, and provides insight to the microscopic mechanisms of transition without recourse to deep understanding or analytical description of atomic dynamics, band structure, electromagnetics, thermodynamics or nanoscale energy conservation.

Cellular automata are fully discrete dynamic systems, wherein each cell of a lattice can exist in one of a finite set of possible states and each cell evolves in each time step according to a set of fixed transition rules dependent upon its initial state and the those of its neighbours. In the present case, each gallium cell can exist in one of three states (Fig. 1a) - a lowest-energy 'ground', higher-energy 'metallic', and a highest-energy, short-lived 'optically excited' state. Ground state optical properties are those of solid α-gallium; optically excited and metallic states present those of liquid gallium. The transition rules applied in each time step are dependent upon the incident photon flux, interface reflectivity (recalculated in each step), rates of thermal and non-thermal excitation from the ground state, metallic and excited state lifetimes, and the phase state of neighbouring cells.

Transition and reflectivity dynamics are found to be controlled predominantly by the relative values of optically-excited and metallic state lifetimes. These determine whether thermal or non-thermal mechanisms dominate and thereby whether the metallization of α-Ga is diffuse (in the short, fs-ps pulse regime – Fig. 1b, c) or proceeds through the motion of a defined solid-liquid melt front (longer pulses). Interestingly, the CA model shows that neighbourhood is essentially irrelevant in the short pulse excitation regime: i.e. at fs timescales there is no coupling between Ga (crystalline) cells, and each cell responds independently to the flux of incident photons.

The cellular automata approach may be applied to a variety phase-change, nonlinear optical and active (nano)photonic systems – for example, the three-level model developed here for Ga may be adapted to VO2, where ultrafast transitions also appear to involve a transient electronically excited state. It has considerable heuristic value for the study of complex nonlinear optical processes and non-equilibrium behaviours in systems close to a transition point, which cannot be described analytically.

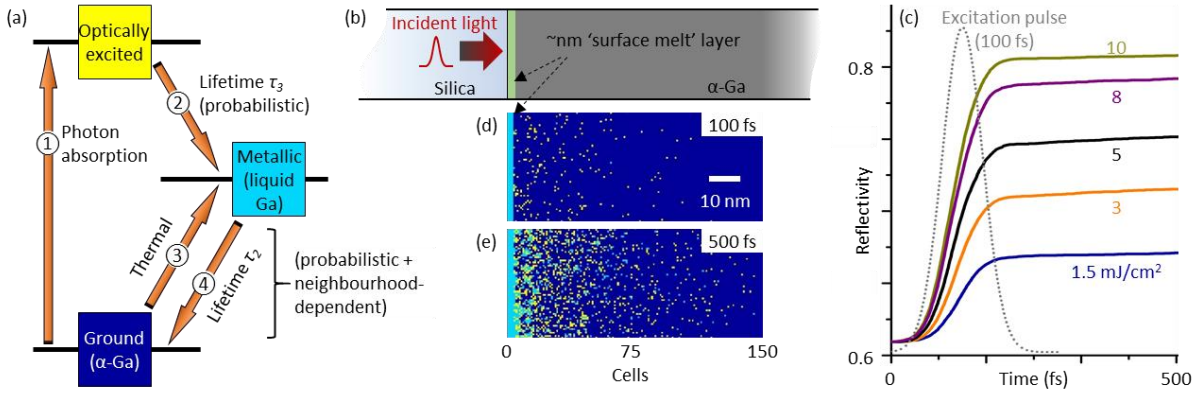

Fig. 1 CA model of Ga-silica interface reflectivity dynamics. (a) Three-level system of Ga cellular automata states and associated transitions ①-④ possible in each time step. (b) Schematic section of the simulated infinite planar Ga/silica interface. (c) Interface reflectivity at 775 nm as a function of time during and immediately after 100 fs pump pulses of varying fluence [as labelled]. (d, e) Representative CA maps of phase state distribution at selected time intervals: (c) during the early part of the pulse; (d) immediately after the pulse.