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Coupling

heat propagation with *lattice vibrations*, *defect dynamics*, and *phase segregation*, in *laser-illuminated* crystalline media: a challenge for the modeler and for the analyst

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in hopes of

pleasing, amusing - and eventually involving -

Professor Gianni Gilardi

on the occasion of his 65th birthday

an on-going joint research project with

Swantje Bargmann (TU Hamburg)

and

Antonino Favata (Rome $\longrightarrow$ TU Hamburg)

PLAN

PART I. LASER INFO

PART II. MODELLING

PART III. ANALYSIS ???

PART I. LASER INFO

LASER

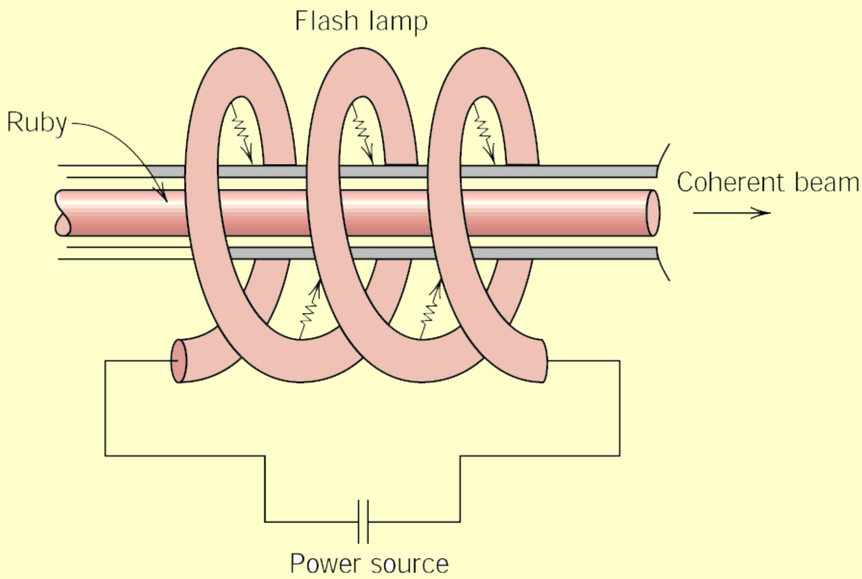
$\equiv$

Light **A**mplification by **S**timulated **E**mission of **R**adiation

- **CW L**aser $\equiv$ **C**ontinuous **W**ave **L**aser, produces a continuous output beam
- **Pulsed L**aser

Principle of Operation

The Ruby Laser. 1/3



- **single crystal of ruby ≡ cromium-doped sapphire** (0.05% Cr^{3-} **ions in** Al_2O_3**, whence the red color); both ends silvered, one tot.**[ly] **reflecting one part.**[ly] **transmitting.**
- **xenon flash lamp**

The Ruby Laser. 2/3

1. ***electrons*** **in Cr atoms are excited into higher energy states by** ***photons*** **from xenon light flash;**

2. **some electrons fall back, others decay to a** ***metastable state*****, where they can reside for up to 3 ms and they hence pile up;**

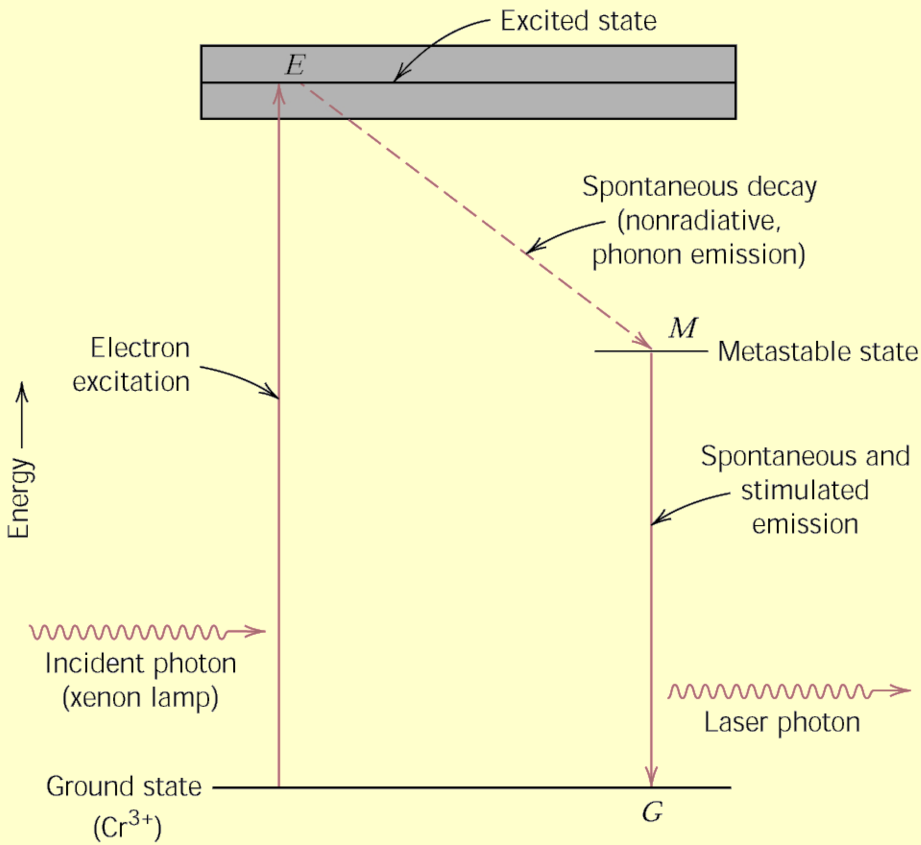
3. **photons spontaneously emitted by few metastable electrons trigger an** ***avalanche of emissions*** **from all the others;**

4. **upon reflection from the silvered ends,** ***photons*** **parallel to the rod's axis stimulate emissions as they travel back and forth;**

5. **finally, an** ***intense, coherent, and highly collimated, light beam*** **is emitted through part.^{ly} silvered end**

   (typical figures: ***wavelenght*** **$\sim 0.7\mu$m, $\sim$ 1 J of** ***energy per pulse*** **of 30 nsec** ***duration*****).**

The Ruby Laser. 3/3



Laser–Matter Interaction

In poor-man solid state physics, L–M interaction is *a play with three types of characters*:

***photons*, *electrons*, and *lattice atoms*;**

the net outcome of their interaction is heating $\equiv$ lattice vibrations.

- **In metals, the *photon*-induced motion of *conduction-band electrons* is damped by collisions with the *lattice*, to which some light energy is transferred.**

- **In semiconductors, the same mechanism involves, in addition to *conduction-band electrons*, also *valence-band holes*.**

- **In dielectrics, *electrons* are effectively bound to the atoms or molecules composing the material: *photons* induce material *polarization*; upon relaxation, some polarization energy is transferred to the *lattice*.**

Applications in Materials Science

Localized heating results in physical changes in matter,

- **undesired (e.g., *laser-induced damage* in optical components),**
- **desired, leading to various types of (*nondestructive testing*, *micromaching*, *biomedical app.s* and) *materials processing*:**
  - ***ablation, vaporization; power cutting; surface hardening;***
  - ***melting* $\Rightarrow$ *recrystallization;***
  - ***annealing* $\Rightarrow$ *attenuation of defect structures*, *in semiconductors and metals*;**
  - ***annealing* $\Rightarrow$ *solid/solid phase transitions* *by atom re-arrangement, in crystalline materials*:**

a business for CGILARDIPS Inc.!

Annealing Ion-Implanted Semiconductors

Ion implantation **induces** ***structural damage*****.**

- **Conventional annealing requires a long heating process in a convection furnace at temperatures over 1000 ^{o}C,**
  - **to remove dislocation networks induced by high-temperature diffusion;**
  - **to reduce misfit defects.**
- **Beginning in the mid-1970s, first in CPPP then in Europe and in the U.S., the use of** ***lasers*** **to anneal** ***silicon wafers*** **was studied, and related** ***modelling activities begun*****.**

PART II. MODELLING

Basic Physical Expectations

When a pulsed laser transfers to crystalline matter a noticeable amount of

***energy, tightly packed in space and time*,**

it may happen that this transfer causes

***thermal and mechanical waves*;**

propagation of these waves may induce

***defect generation/annihilation* and *solid/solid phase transitions*.**

What We would Like to Study is

how pulsed-laser heating influences

- lattice vibrations
- defect dynamics
- phase segregation

To do this, . . .

. . . we must build on the Four Pillars of Wisdom:

- **(internal) energy balance**
- **momentum balance**
- **concentration balance**
- **order-parameter balance**

and we must

capture the target phenomenology by thermodynamically consistent constitutive choices*, to be made *standing on the top of

the Fifth Pillar:

- **entropy imbalance.**

What has been done so far

Each of the four basic evolution phenomema:

- ***thermal conduction, thermal waves***
- ***lattice straining, mechanical waves***
- ***defect dynamics***
- ***phase segregation***

can be and has been studied *per se*. Let's exemplify how . . .

- ***thermal conduction, thermal waves***

  energy balance + constitutive choices imply:

  $$\text{either} \quad \dot{\vartheta} = \kappa\Delta\vartheta + r \quad \text{or} \quad \tau\ddot{\vartheta} + \lambda\dot{\vartheta} = \kappa\Delta\vartheta + r$$

- ***lattice straining, mechanical waves***

  momentum balance + linear elasticity package imply:

  $$\rho\,\ddot{\boldsymbol{u}} = \mu\Delta\boldsymbol{u} + (\lambda+\mu)\nabla\,\mathbf{Div}\,\boldsymbol{u} + \boldsymbol{d}$$

- ***defect dynamics***

  concentration balance + constitutive choices about diffusion and generation/annihilation imply:

  $$\dot{n} = \gamma\Delta n + d(n)$$

- ***phase segregation***

  standard variational deductions of gradient-flow style imply:

  $$\text{(A-C)} \quad \beta\,\dot{\rho} = \alpha\,\Delta\rho - f'(\rho), \quad \text{(C-H)} \quad \dot{\rho} = \kappa\,\Delta(f'(\rho) - \alpha\Delta\rho$$

(for a P-of-W deduction, see CGILARDIPS papers)

Attempted Couplings. 1/2

- *heat conduction* + *mechanical waves*

  led to various theories of *thermoelasticity* (see B. Straughan's *Heat Waves*, Springer, 2011), some (the roughest ones) tailored for laser-heating situations (Wang & Xu, 2002). A *doubly hyperbolic* theory remains to be put together.

- *mechanical waves* + *defect dynamics*

  led to the work of *Mirzade* (2011) (Institute on Laser and Information Technologies, Moscow) and coworkers:

$$\rho \ddot{\boldsymbol{u}} = \mu \Delta \boldsymbol{u} + (\lambda + \mu) \nabla e(\boldsymbol{u}) - \vartheta_d \nabla n, \quad e(\boldsymbol{u}) = \mathbf{Div}\, \boldsymbol{u},$$
$$\dot{n}_1 = D \Delta n_1 - \vartheta_d\, g_d(T) \Delta e(\boldsymbol{u}) - \tau^{-1} n_1 + \widetilde{g}_d(T)\, e(\boldsymbol{u}).$$

Note the structure of the *concentration (not segregation!) PDE*:

$$\dot{n} = -\mathbf{Div}\, \boldsymbol{d} + d, \quad \boldsymbol{d} = \boldsymbol{d}_{dif} + \boldsymbol{d}_{adv}.$$

In all these works, *temperature is a parameter*. A theory where temperature evolves is badly wanted.

Attempted Couplings. 2/2

- *strain* + *phase segregation*

  (see, e.g., Fried & Gurtin, 1993, and Gurtin, 1996). This attempt seems worth further pursue.

- standard *heat conduction* + P-of-W *A-C phase segregation*

  (see CGILARDIPS, Adv. Math. Sci. Appl., 2010).

A New & Enticing Coupling

hyperbolic ***heat conduction***

$+$

P-of-W ***A-C phase segregation***

Thank you for your kind attention!

Happy Birthday GG!