Introduction

Useful forms of energy. Since diffuse (ca. 170 Wm⁻²) current, conversion should integration and storage. Curve of the many routes used to energy into heat, electricity is competitive with fossil fuel's world market price.

"Over 50% of energy use in modern houses is spent in warming up water for heating, washing, and cooking."

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The efficiency of the collector depends crucially on: the **selectivity** (solar absorbance / thermal emittance), and the **stability** (high operating temperatures) of the absorber.
Diamond-like carbon (DLC) is tough with suitable optical gap

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- **a-C, bulk modulus**: bulk modulus $B\text{_{sp}}$ as a function of coordination $z$
- **a-C, optical gap**: optical gap as a function of sp$^3$ fraction (%)
- **a-C:H/Au, TEM image**: image of a-C:H/Au
- **DLC with metal, absorption**: absorption coefficient as a function of wavelength (nm)

Simulation and design of metal-containing DLC

Structural models

Properties
- Structural
- Electronic
- Optical
- Mechanical
Structural models

Models of 70-100% sp$^3$ DLC and Ag/Cu-DLC

sp$^3$-bonded C

sp$^2$-bonded C

PBEsol DFT for structural optimization

“amorphous diamond”

3% at. Me - DLC
Graphitization of DLC with metal incorporation: 7% decrease in sp³-bonded C for 1% increase in metal content

\[ \Delta \text{sp}^3 \] (\%)

\[ \text{[Me]} \] (% at.)

\[ \text{sp}^3 \] (\%)

**Theory**

**Experiment**¹

\[ \text{Slope: } \sim -8.5\% \]

Electronic properties

The metallic inclusions introduce states into the DLC band gap

\[ w(\epsilon) = \sum \left( \frac{N g_i(\epsilon)}{g(\epsilon) - 1} \right)^2 / N(N-1), \quad g_i: \text{PDOS on atom } \text{“i”} \]
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\[ \text{model a-C}^1 \]

Optical properties

Metal incorporation in DLC enhances absorption in the visible

Time-dependent DFT (Bootstrap approximation for the xc kernel)

Metal incorporation in DLC softens the material

Finite deformation (stress-strain) approach
Metal incorporation in DLC enhances absorption in the visible; The composite softens but retains good mechanical strength

\[ \sim 1.6 \times 10^3 \text{ cm}^{-1} / 5\% \text{ sp}^2 \]

\[ \sim 10 \text{ GPa} / 5\% \text{ sp}^3 \]
Design of metal-containing DLC
DLC with 70-80% sp³-bonded C and < 3% at. metal shows high absorption in the visible ($\alpha > 10^5 \text{ cm}^{-1}$) and good mechanical strength ($\kappa > 300 \text{ GPa}$, $\gamma > 500 \text{ GPa}$)

Georgios A. Tritsaris, Christos Mathioudakis, Pantelis C. Kelires, and Efthimios Kaxiras, Submitted

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