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COMSOL Multiphysics Simulations of Graphene Chemical Vapor Deposition (CVD) Growth

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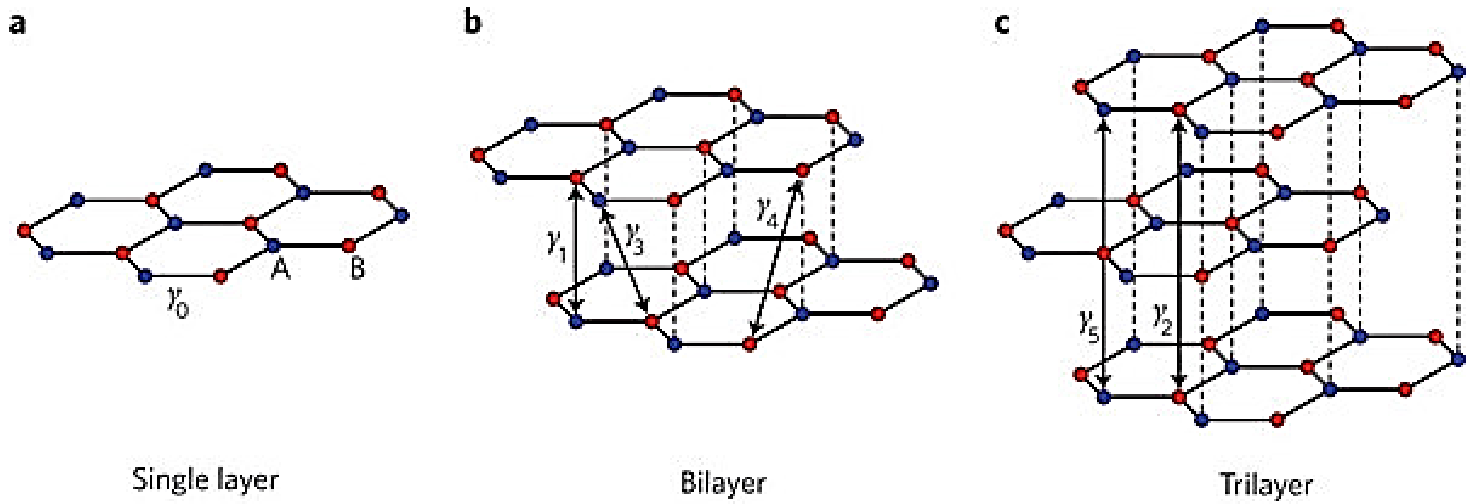
Outline

- Graphene and Graphene properties
- COMSOL Multiphysics Simulations of Graphene CVD Growth Mechanism Using Cu
- COMSOL Computational Methods
- Simulated Results and Discussion
- Conclusion

What is graphene?

Graphene is a single atomic layer, first isolated in 2004, organized in a two dimensional hexagonal (honeycomb) lattice structure



Weak Van der Waals forces

Graphene (sp2 bonded carbon atoms)

The carbon-carbon bond length in graphene is approximately 0.142 nm.

Graphite

Graphite itself consists of many graphene sheets stacked together

Graphene Properties

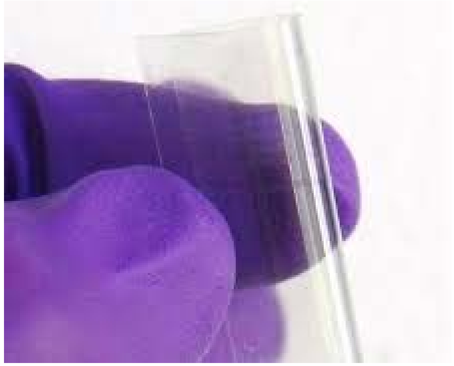
- The thinnest and lightest material known

  (1 m^2 ~ 0.77 mg)
- The strongest material discovered

  (100-300 times stronger than steel)
- The best conductor of electricity and heat

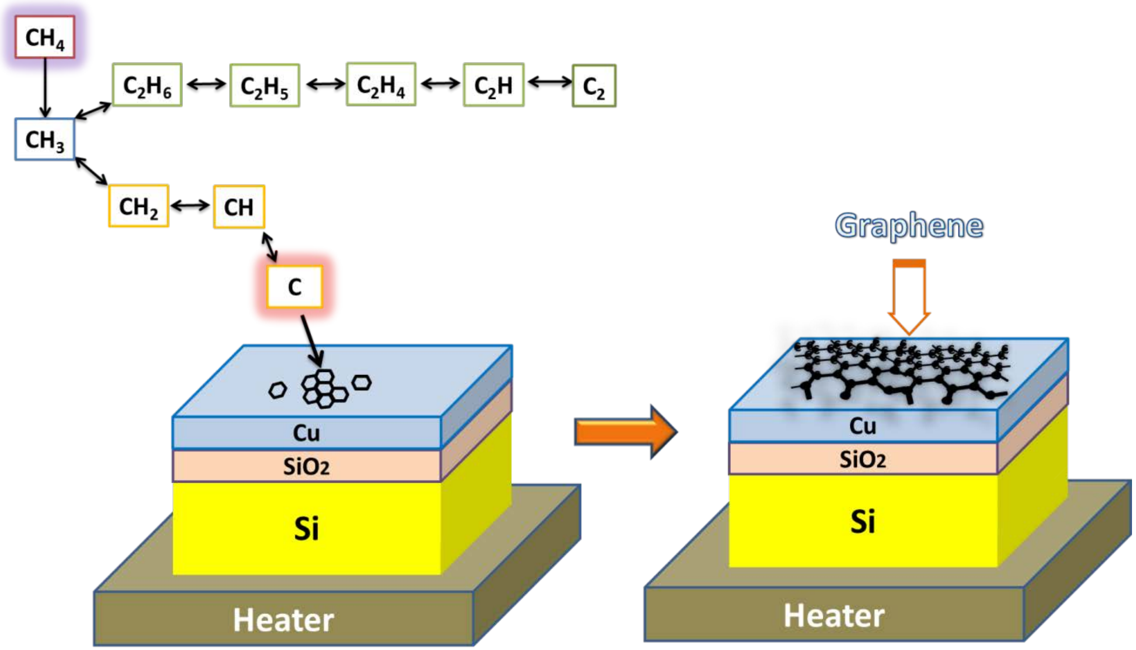
  Extremely high mobility of electrons

  (more than2.0 x 10^5 at room temperature (cm^2 V^{-1} s^{-1})
- Graphene absorbs approximately 2.3% of white light.

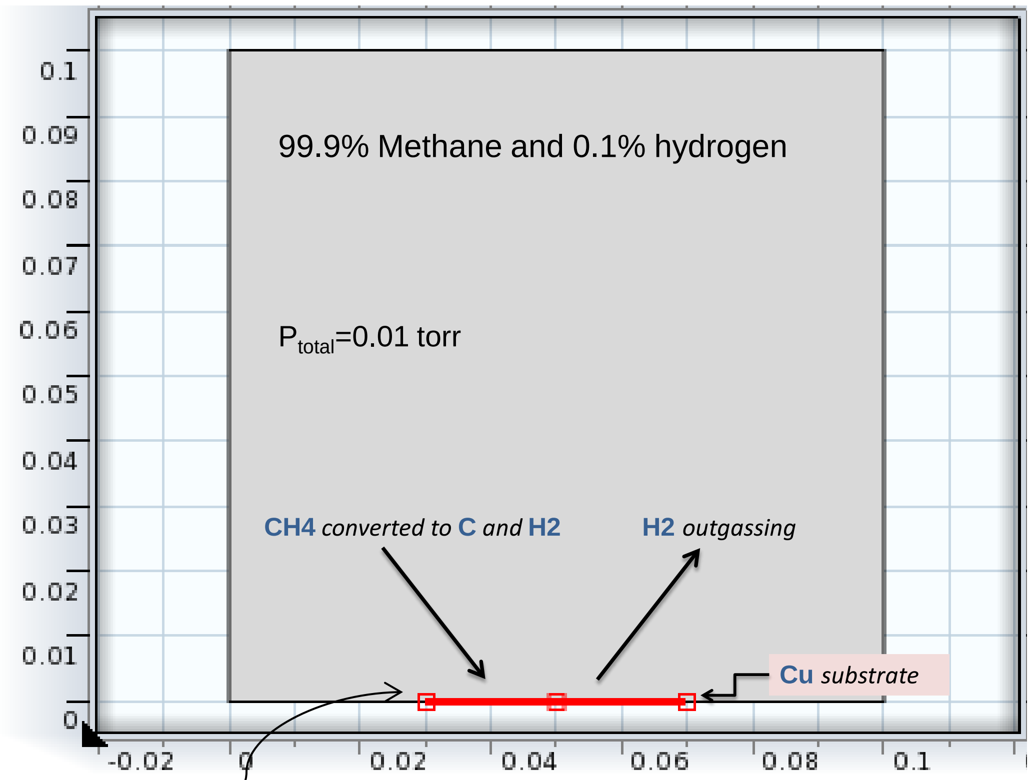


Graphene CVD Growth Mechanism Using Cu

Graphene CVD growth process on Cu thin film



Computational Methods



T=700 °C

Computational Methods

COMSOL model uses ***Laminar Flow, Heat Transfer, and Heavy Species Transport*** application in order to investigate:

- CH_4 decomposition reactions encountered in the CVD chamber.
- Graphene growth on Cu surface.

$$CH_4 + 5S_{(Cu)} \rightarrow \text{graphene}_{(a)} + 2H_{2(g)}$$

$$r_i = k_i^f \prod_{k=1}^{K} c_k^{v_{ki}^f}$$; The surface reaction rate

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \boldsymbol{u}) = 0$$; The continuity equation

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u}.\nabla u = -\nabla \boldsymbol{p} + \nabla.\left(\mu(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T) - \frac{2}{3}\mu(\nabla.\boldsymbol{u})\boldsymbol{I}\right)$$; The momentum balance equation

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{u}.\nabla T = \nabla.(\kappa \nabla T) + Q$$; The energy balance equation

$$\boldsymbol{u} = -\frac{M_f}{\rho}\boldsymbol{n} \qquad M_f = \sum_{k=1}^{K_g} M_k \dot{s}_k \qquad \dot{s}_k = \sum_{i=1}^{I} V_{ki} r_i$$

The average velocity of the mass species

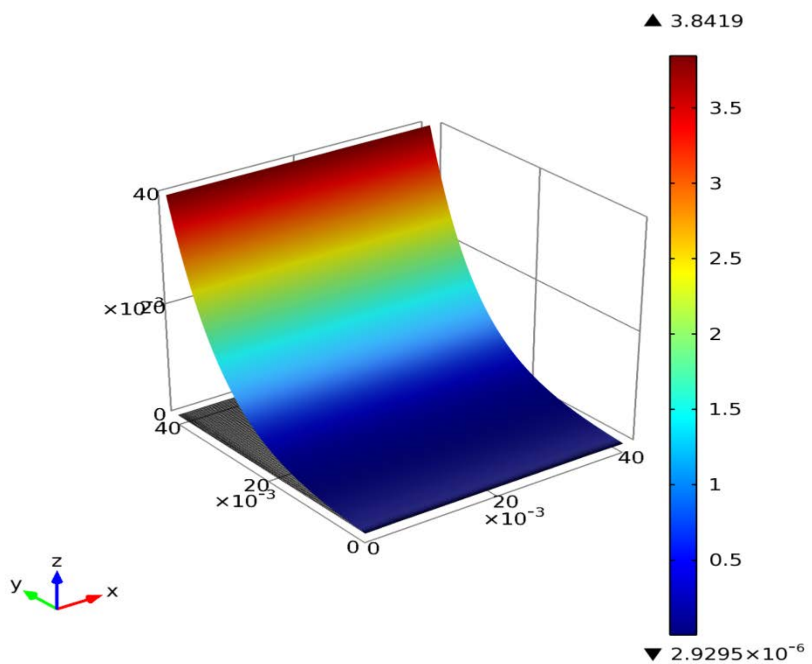
The mass flux

The surface rate expression

Results

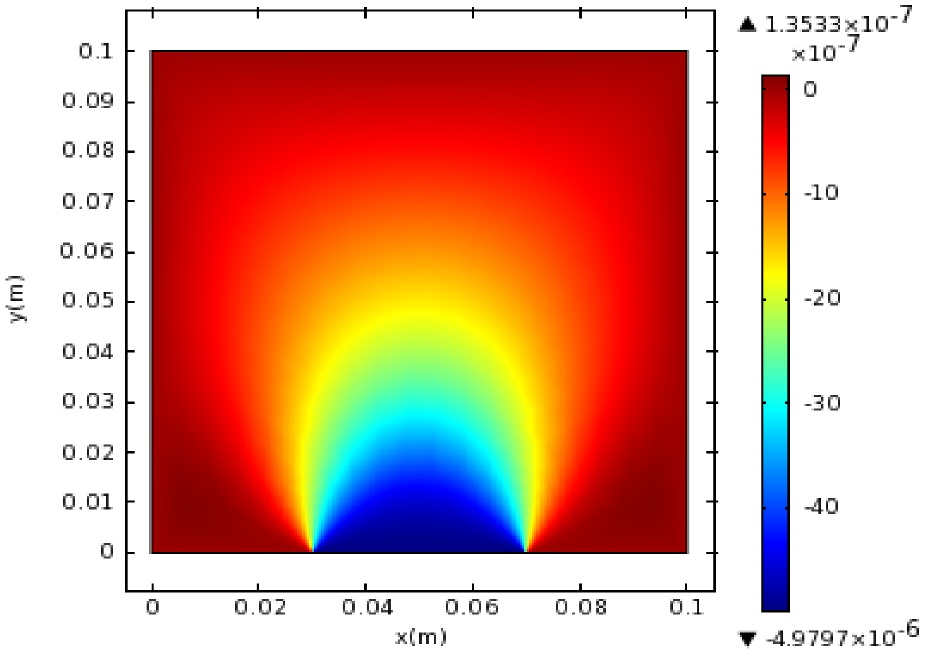
Accumulated graphene growth height (Å) after 1300 sec at H_2 fraction equals 0.001.

T=700 °C
P= 0.001 torr



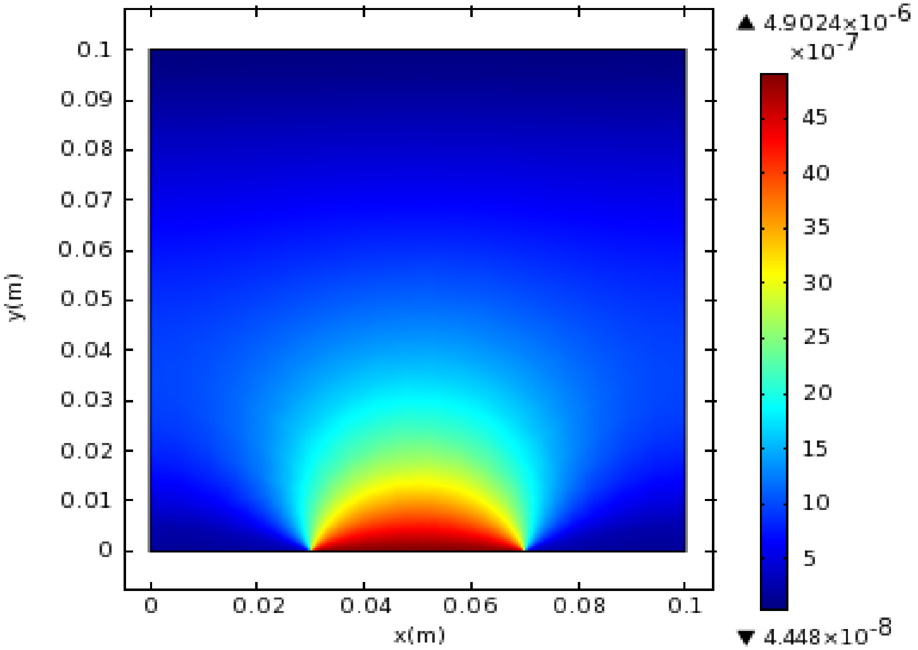
Results

The y- component of the mass averaged velocity at=10 s.



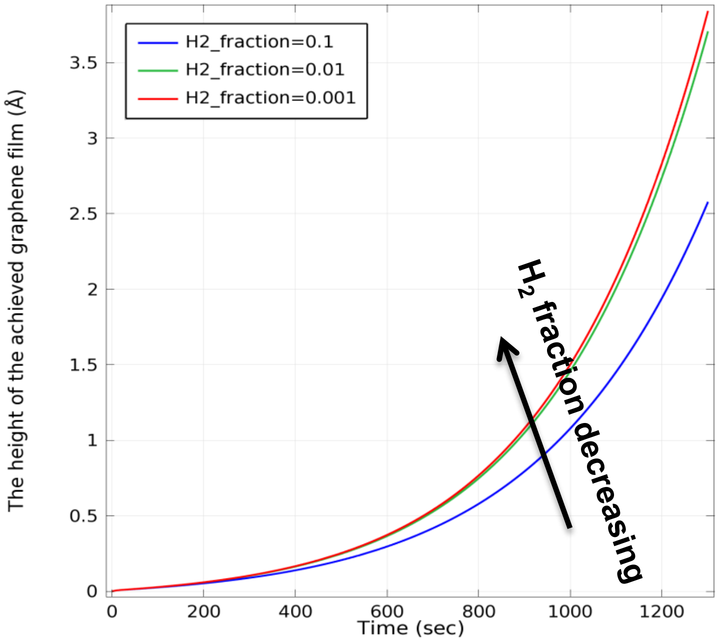
Results

The y- component of the diffusion velocity for hydrogen at=10 s.



Results

The influence of the H_2 fraction upon graphene film thickness .



Conclusion

- CVD graphene growth on Cu thin films by direct deposition process has modeled using COMSOL MULTIPHYSICS.
- ***Laminar Flow, Heat Transfer, and Heavy Species Transport*** application were utilized to simulate graphene chemical vapor deposition (CVD) growth process on Cu.
- ***Monolayer graphene*** film was achieved by methane decomposition at 700 °C where the total pressure equals ~ 0.01 torr..
- This model can be extended to simulate graphene growth using different catalysts as well as different carbon precursors.

Thanks

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