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UNIVERSITY OF ARKANSAS

CVD Graphene Growth Mechanism on Nickel Thin Films

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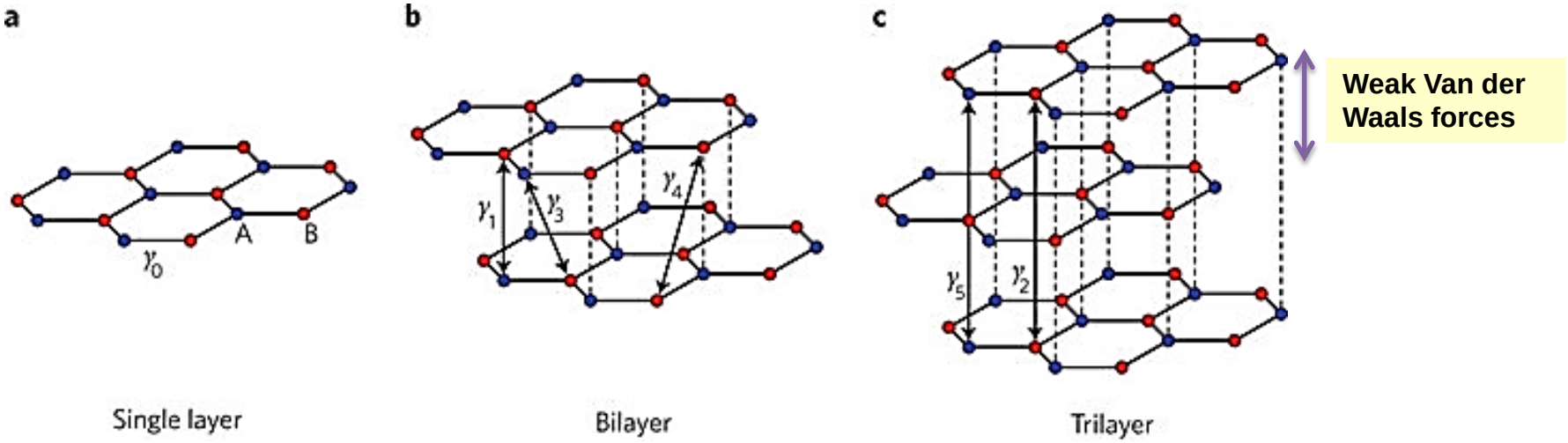
Outline

- Graphene and Graphene properties
- COMSOL Multiphysics Simulations of Graphene CVD Growth Mechanism Using Ni
- 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



Graphene (sp2 bonded carbon atoms)

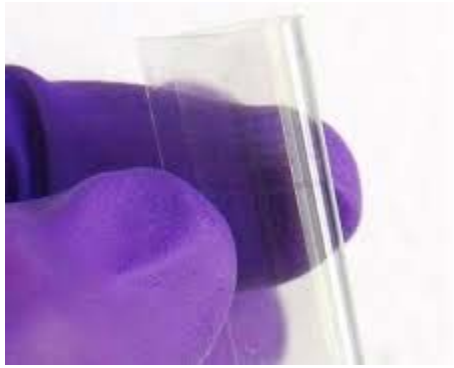
The carbon-carbon bond length in graphene is approximately 0.142 nm.

Graphite

Graphite itself consists of many graphene sheets stacked together

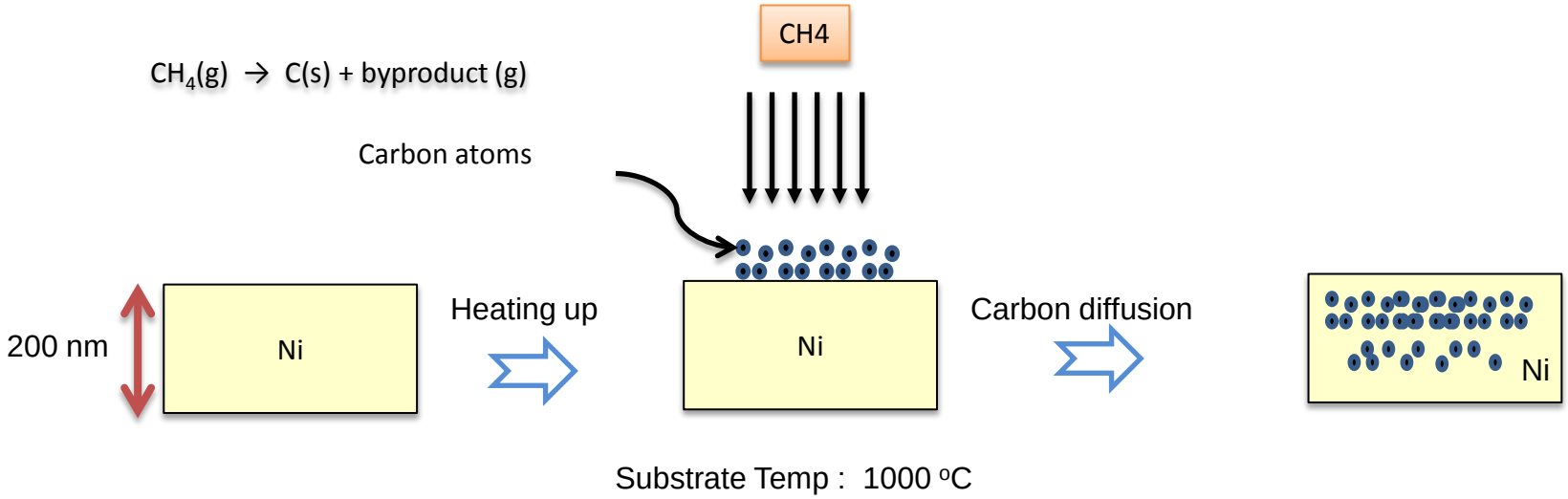
Graphene Properties

- 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.

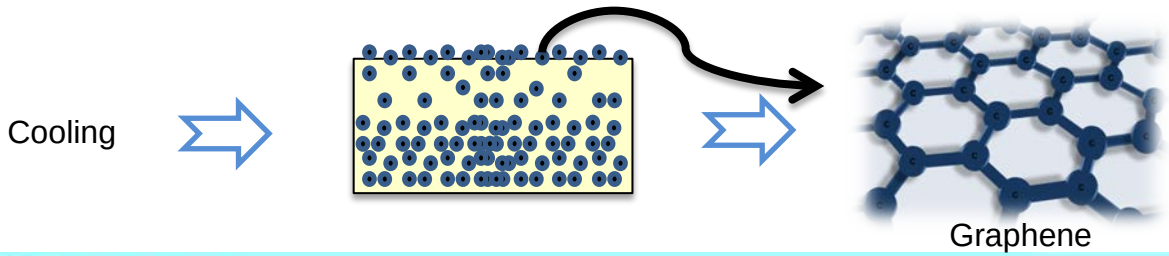


Graphene CVD Growth Mechanism Using Ni

A. Carbon diffuses into Ni (Dissolution Mechanism)



B. Carbon precipitate on Ni surface due to cooling process (Precipitation Mechanism)



Computational Methods

Heat transfer, mass transfer, and deformed geometry applications were employed to simulate :

- CVD graphene growth on nickel thin film by dissolution-precipitation mechanism
- calculate the number of achieved graphene layers.

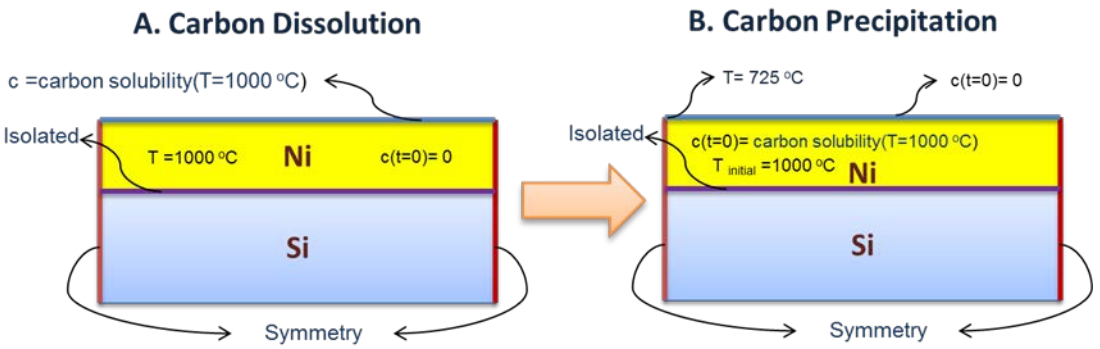
$$\frac{\partial c}{\partial t} = \nabla.(D\nabla c)$$

$$\rho C_P \frac{\partial T}{\partial t} = \nabla.(\kappa \nabla T)$$

$D = D_0 \exp(-E_D/kT)$ (in $cm^2 .s^{-1}$)

$S = S_0 \exp(-H_0/kT)$ (in atoms.cm−3)

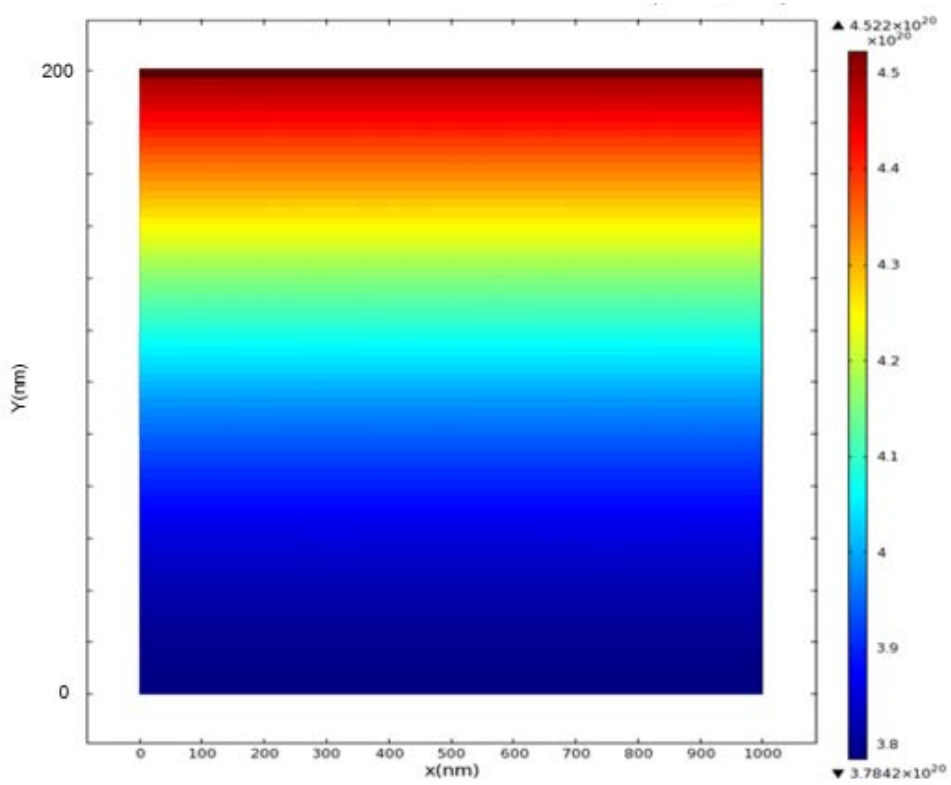
$$v_y = \frac{\vec{J}_m.\hat{n}_y}{\rho_{carbon}}$$



Results

A. Dissolution Stage

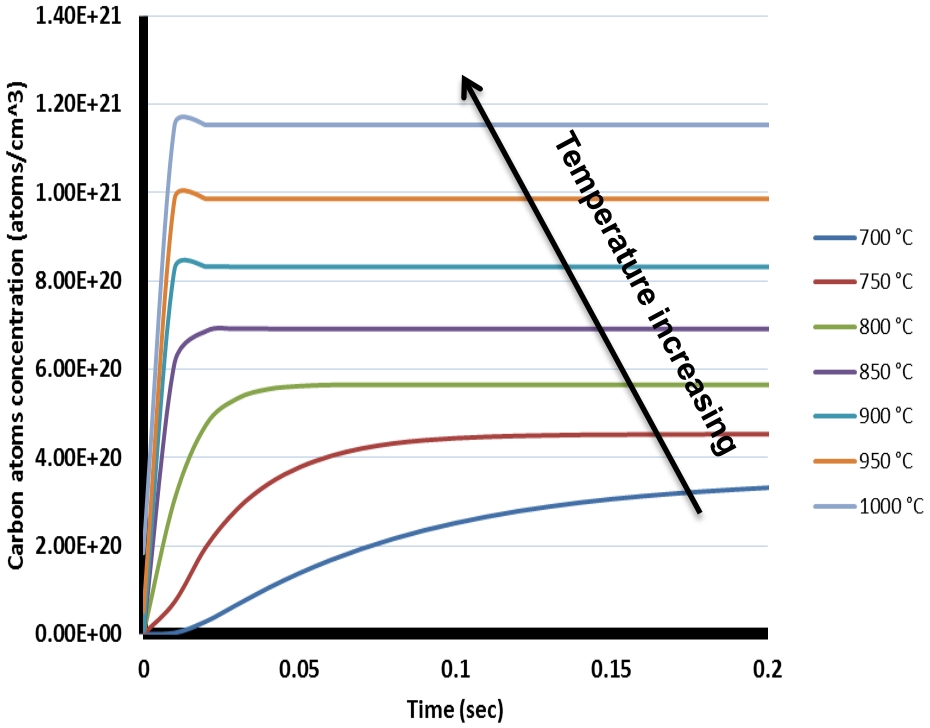
Carbon atoms diffusion field at 0.05 sec inside 200 nm thick nickel film at 1000 ° C

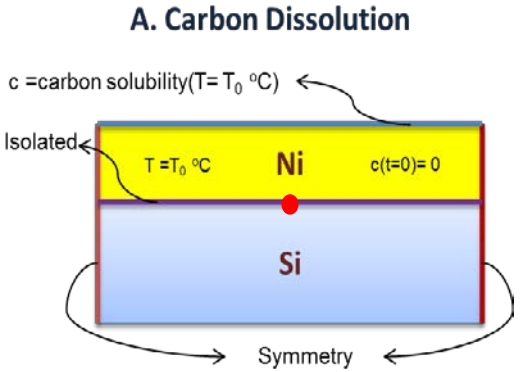


Results

A. Dissolution Stage

The influence of temperature on carbon atoms concentration at the bottom side of the Ni film.

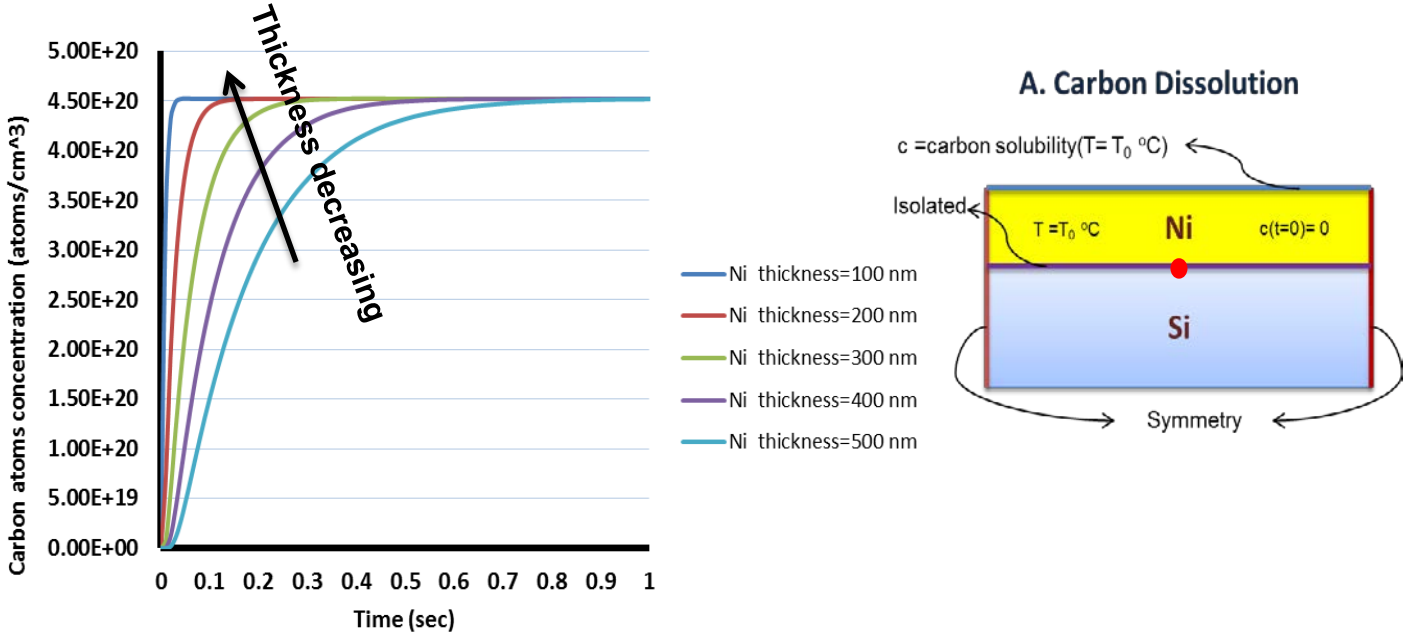




Results

A. Dissolution Stage

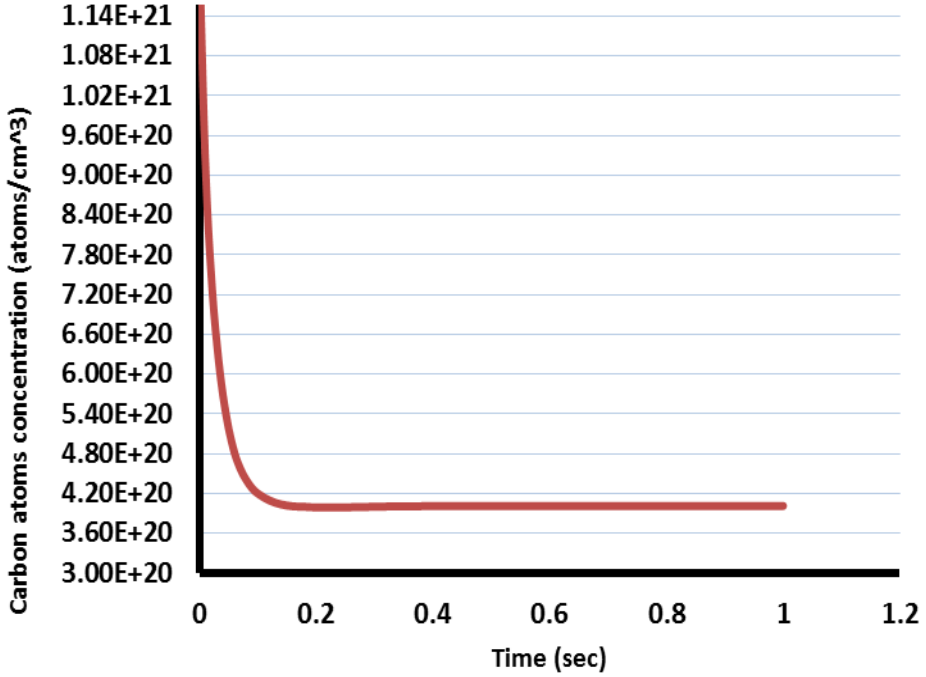
The influence of the Ni film thickness upon carbon atoms saturation at 1000 °C. .

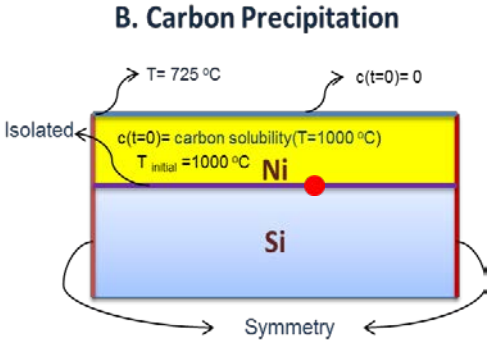


Results

B. Precipitation Stage

The outward carbon atoms diffusion driven by **supersaturation** in the Ni film when the Ni film temperature drops from 1000 °C to 725 °C.

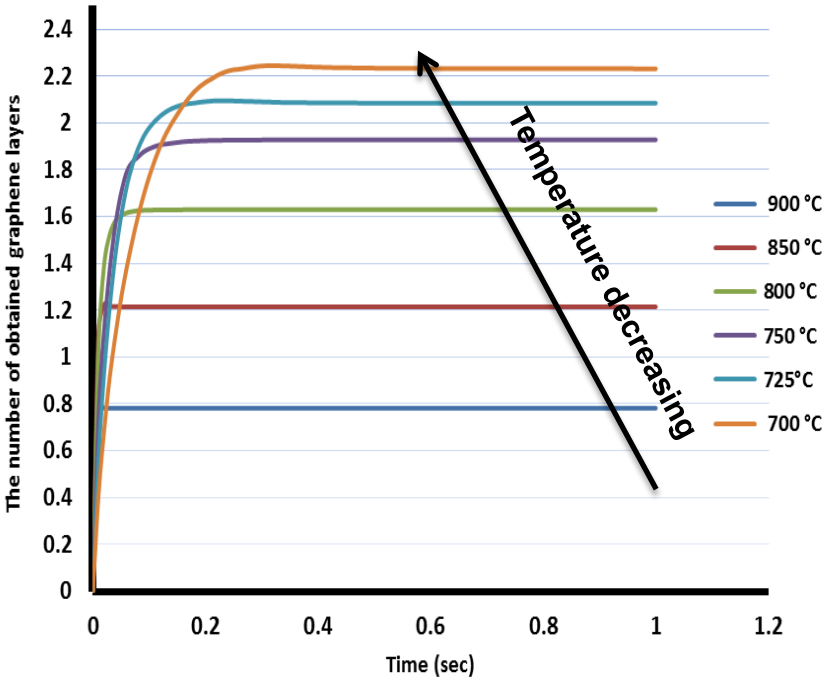


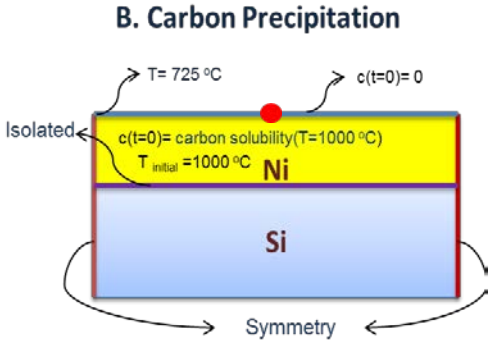


Results

B. Precipitation Stage

The number of the obtained graphene layers on Ni film surface after cooling from **1000 °C to different temperature**



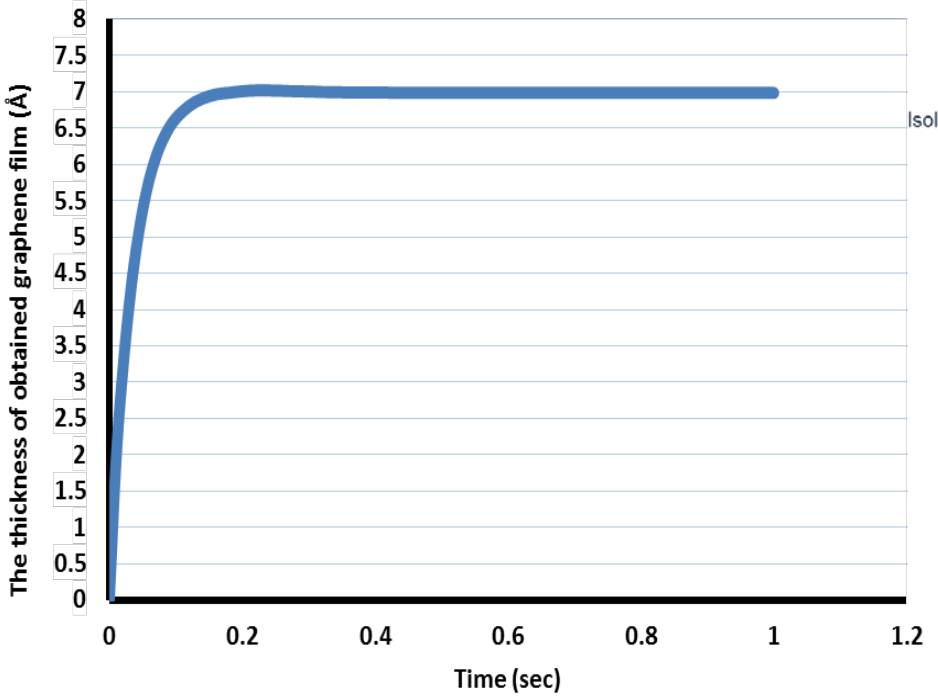


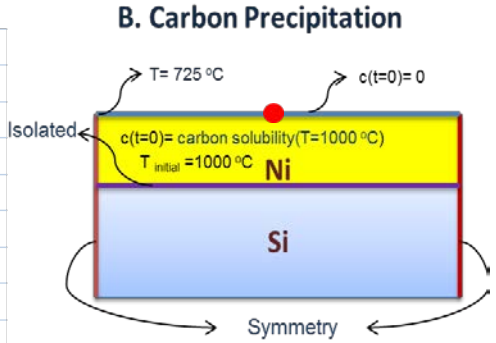
Results

B. Precipitation Stage

The thickness of the obtained graphene film on Ni film surface after cooling from **1000 °C to 725 °C**.

Two Layers of Graphene

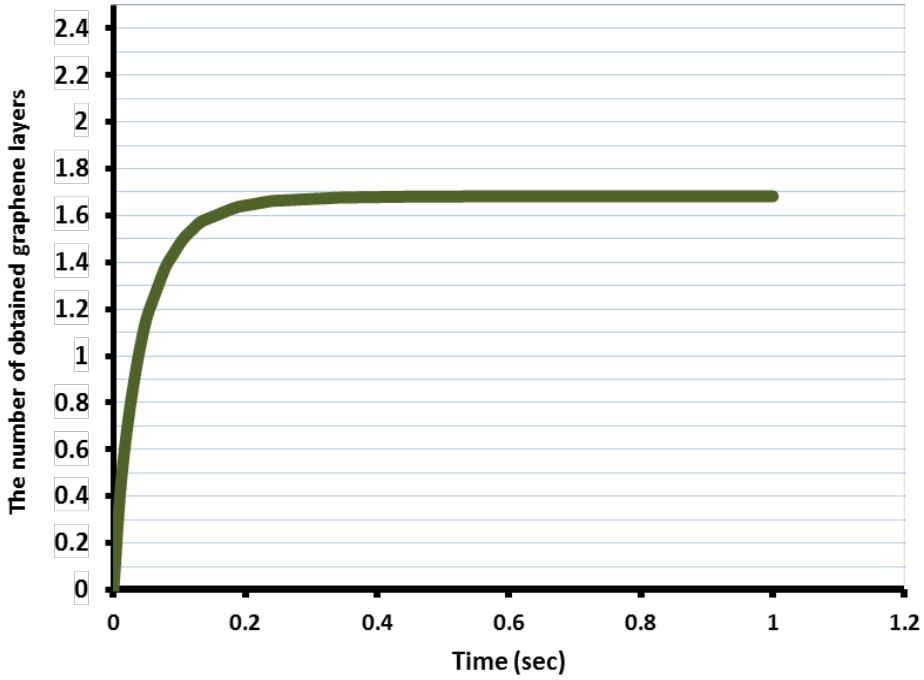


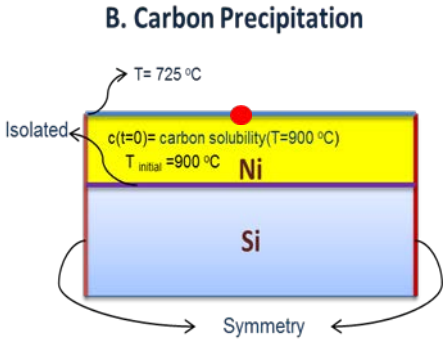


Results

B. Precipitation Stage

The number of the obtained graphene layers on Ni film surface after cooling from **900 °C to 725 °C**.





Accuracy Check

- Baraton et al. had conducted an experiment typical to the one that we have modeled.

- The experimental work of Baraton et al., in terms of the number of graphene layers, is similar to the obtained value (**1.7 layers)** in our simulation utilizing COMSOL MULTI PHYSICS software.

Conclusion

- CVD graphene growth on nickel thin films by dissolution- precipitation mechanism has modeled using COMSOL MULTIPHYSICS.
- *Heat transfer*, *mass transfer*, and *deformed geometry* models were employed to simulate inward and outward carbon atoms diffusion in the Ni film as well as the number of achieved graphene layers.
- Cooling 200nm thick Ni film saturated with carbon atoms from 900 °C to 725 °C leads to precipitate ***1.7 graphene layers*** on the Ni film surface.
- The obtained number of graphene layers was compared with a real experimental data.
- We have found that COMSOL results are reasonable.

Thanks