CVD Graphene Growth Mechanism on Nickel Thin Films

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Introduction: Chemical vapor deposition is considered a promising method for synthesis of graphene films on different types of substrate utilizing transition metals such as Ni. However, synthesizing a single-layer graphene and controlling the quality of the graphene CVD film on Ni are very challenging due to the multiplicity of the CVD growth conditions. COMSOL Multiphysics is used to investigate the graphene CVD growth on Ni film and determine the main factors affecting graphene CVD synthesis. Our COMSOL model uses transport of diluted species, heat transfer in Ni thin film as well as deformed geometry. In this particular research, the number of the simulated graphene layers on Ni film is compared with experimental data.

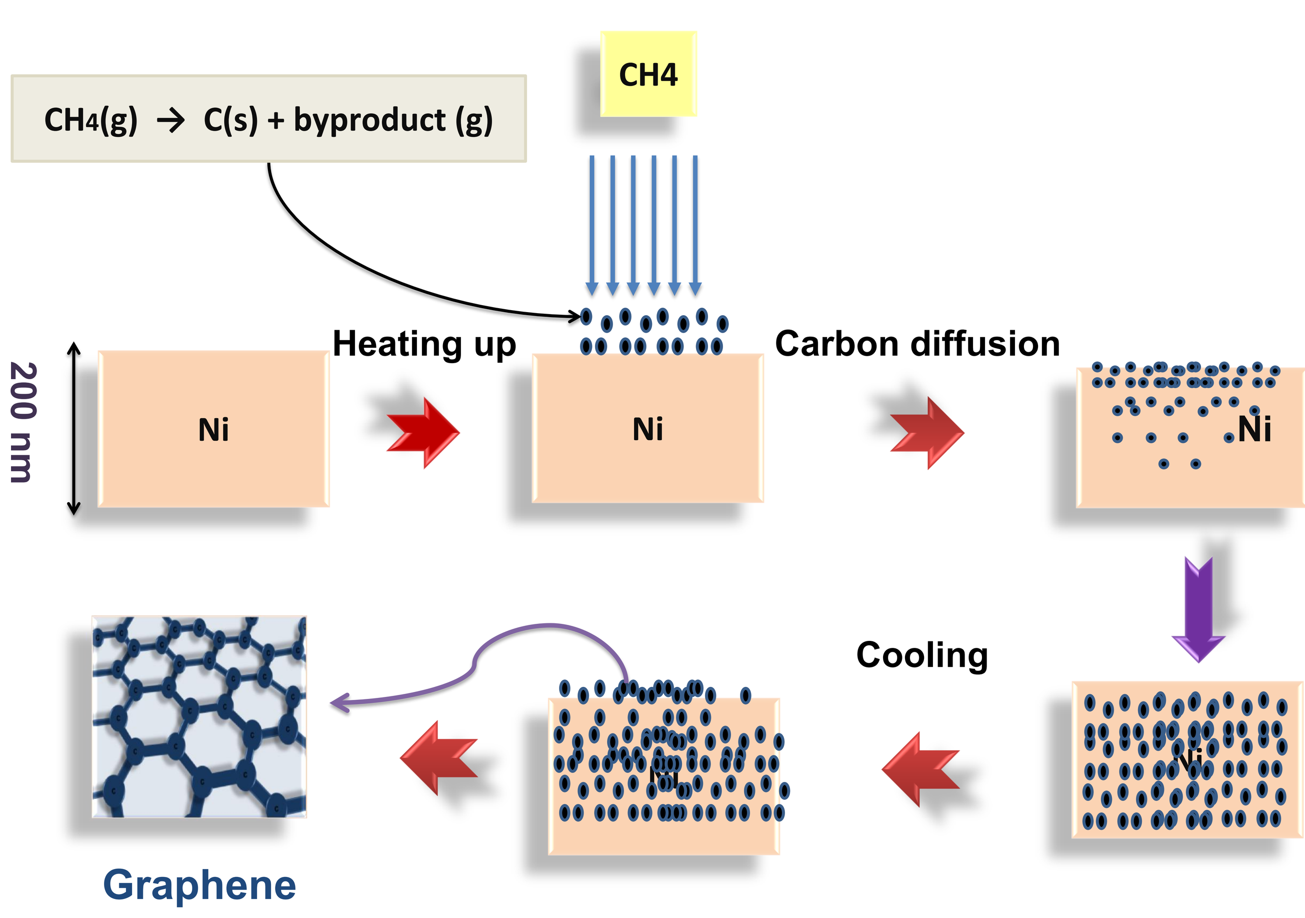

Figure 1. CVD graphene growth mechanism on nickel.

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 as well as to calculate the number of achieved graphene layers.

$$\frac{\partial c}{\partial t} = \nabla.(D\nabla c) \qquad \rho C_p \frac{\partial T}{\partial t} = \nabla.(k\nabla T)$$

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

$$S = S_0 \, exp\,(H/kT) \ \ (\text{in atoms.cm}-3)$$

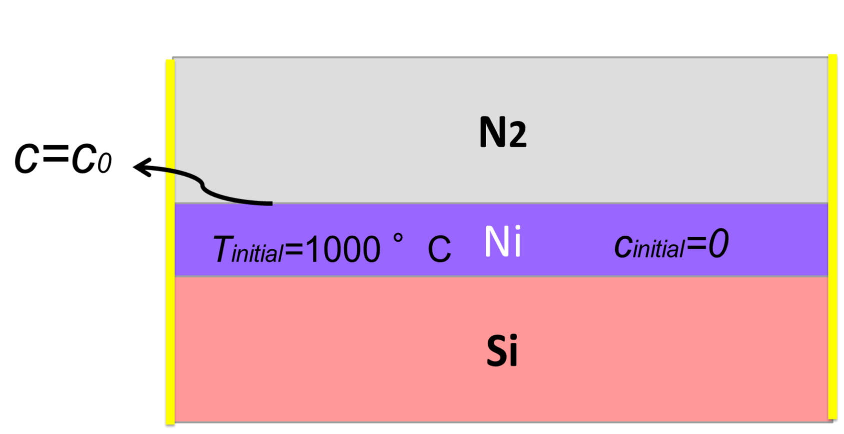

Figure 2. Boundary conditions within carbon dissolution period.

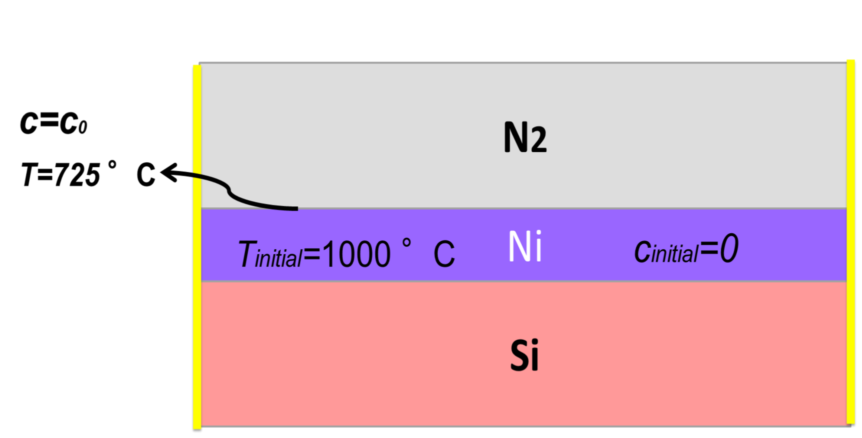

Figure 3. Boundary conditions within carbon precipitation period.

Results:

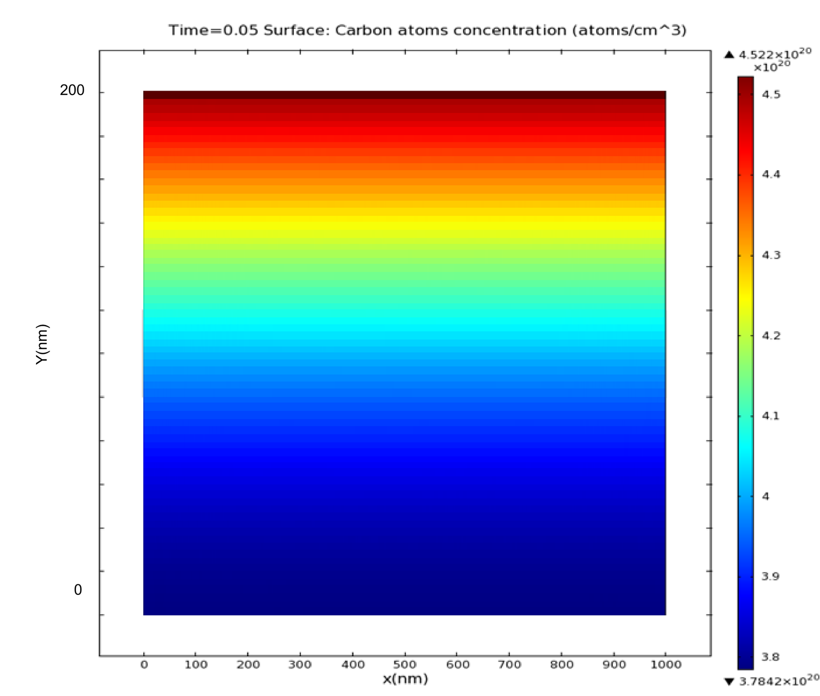

Figure 4. Calculated carbon atoms diffusion field inside 200 nm thick nickel film.

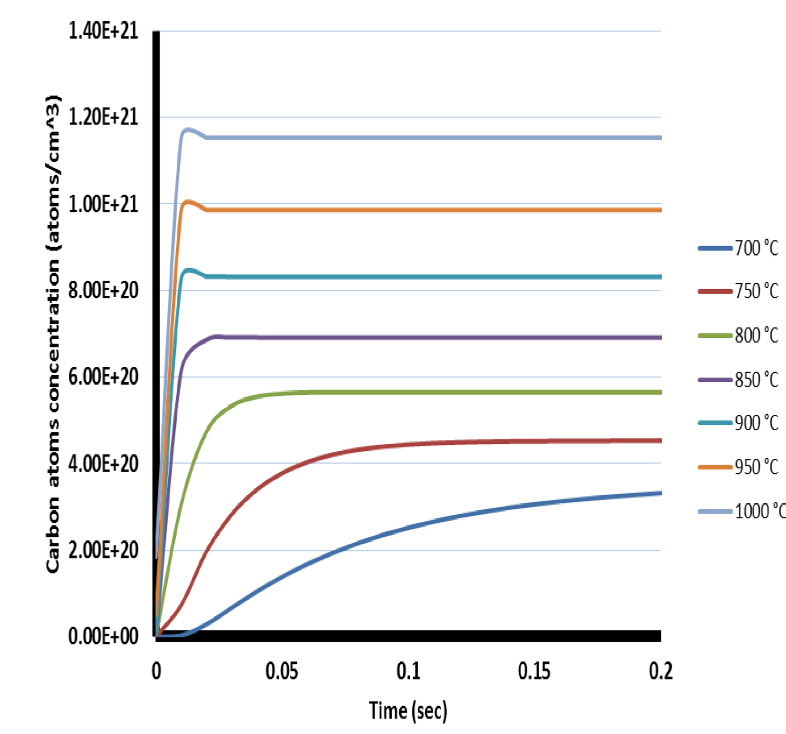

Figure 5. The influence of temperature on carbon atoms diffusion inside the Ni film.

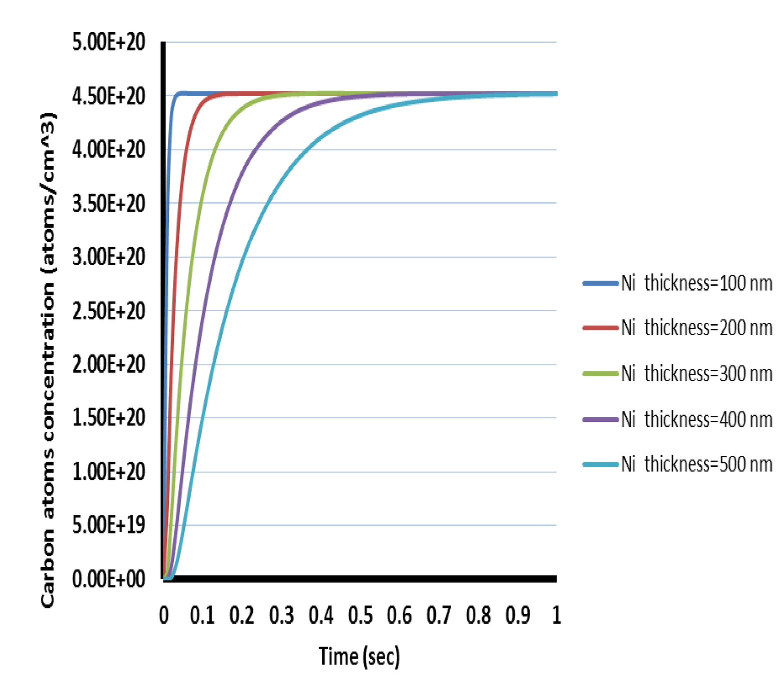

Figure 6. The influence of the Ni film thickness upon carbon atoms saturation.

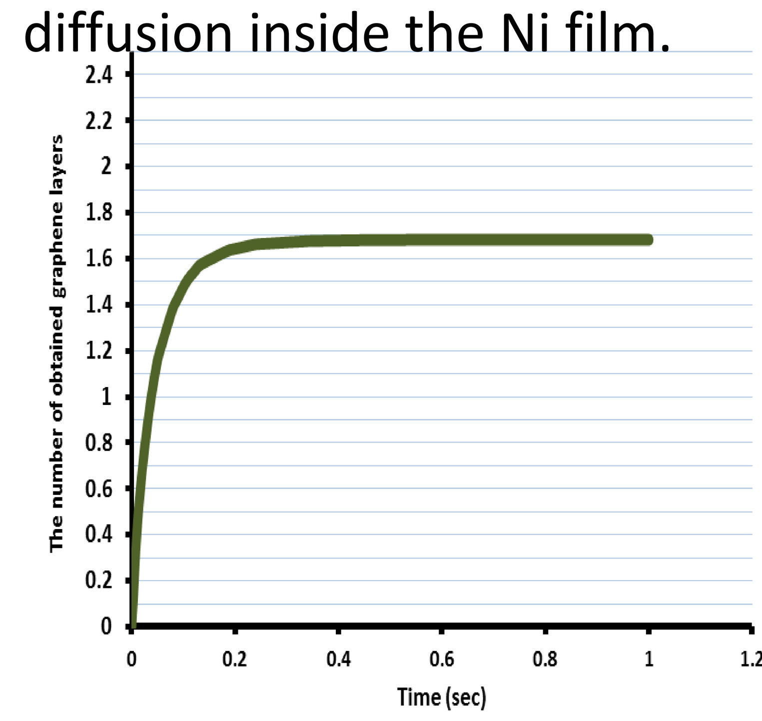

Figure 7. The number of the obtained graphene layers on Ni film surface after cooling from 900 ° C to 725 ° C.

Conclusions: CVD graphene growth on nickel thin films by dissolution- precipitation mechanism has modeled using COMSOL. To explain, Heat transfer, mass transfer, and deformed geometry applications were employed to simulate inward and outward carbon atoms diffusion in the Ni film as well as the number of achieved graphene layers. The obtained number of graphene layers was compared with experimental data. We have found that COMSOL results are reasonable.

References:

1. Baraton L, On the mechanisms of precipitation of graphene on nickel thin films. EPL (Europhysics Letters) 2011;96(4):46003.
2. Reina A, Kong J. Graphene growth by CVD methods. In: Graphene nanoelectronics. Springer; 2012.
3. Meyer JC, Geim AK, Katsnelson M, Novoselov K, Booth T, Roth S. The structure of suspended graphene sheets. Nature 2007;446(7131):60-3.
4. Li X, Magnuson CW, Venugopal A, Tromp RM, Hannon JB, Vogel EM, Colombo L, Ruoff RS. Large-area graphene single crystals grown by low-pressure chemical vapor deposition of methane on copper. J Am Chem Soc 2011;133(9):2816-9.