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Chemical Vapour Deposition Reactor Design for Graphena Synthesis

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Abstract: A graphene is a important material for electronic application and others such as battery, resistant corrosion coating, and biosensor. There was some technics for graphene synthesis among others reduction graphite oxide method, adhesive tape, and chemical vapour deposition (CVD). The CVD technic produced a more excellent graphene materials than others although more expensive in the production process. In this research scopes were developed a CVD which designed by Ansys and Hysys simulation. The results shown the caviler copper pipes have a strenght tube about 0.1 Mpa then the pressure simulation can be achieved use pipes diameter 0.25 mm was 1.013 x 105 Pa. CVD reactor have a minium power at 4500 kJ/hr to operation condition at a length of 10 cm and the formation of graphene at a tube length of 40 cm.

Keywords: Graphene, chemical vapour deposition, advance material, entrophy, hysys.

Abstrak: Graphene adalah material penting untuk aplikasi elektronik dan lain-lain seperti baterai, lapisan tahan korosi, dan biosensor. Ada beberapa teknik untuk sintesis graphene antara lain metode reduksi grafitoksida, pita perekat, dan deposisi uap kimia (CVD). Teknik CVD menghasilkan bahan graphene yang lebih unggul dari yang lain meskipun lebih mahal dalam proses produksinya. Dalam ruang lingkup penelitian dikembangkan CVD yang dirancang dengan simulasi Ansys dan Hysys. Hasil penelitian menunjukkan pipa tembaga caviler memiliki kekuatan tabung sekitar 0,1 Mpa kemudian simulasi tekanan dapat dicapai menggunakan pipa berdiameter 0,25 mm adalah 1,013 x 105 Pa. Reaktor CVD memiliki daya minium sebesar 4500 kJ / jam untuk kondisi operasi pada panjang pipa. 10 cm dan pembentukan graphene pada panjang tabung 40 cm.

Kata kunci: Graphena, chemical vapour deposition, material maju, entropi, hysys.

INTRODUCTION

A Chemical Vapour Deposition (CVD) has been developed to produce advance material for electronic manufacturing in several industry sector. In a practical and common definition of CVD is that it is complex process of depositing solid materials at a high temperature as a result of a chemical reaction. This deposition forms a special type of material commonly known as ordered crystal grow from vapour [1]. Graphene is a monolayer sheet recently fabricated [2-4] and has been attracting attention theoretically and experimentally since the observation of integer quantum hall effect [2,3,4].

Several techniques have been established for graphene synthesis such as Mechanical cleaving (exfoliation) (Novoselov et al. 2004), chemical exfoliation (Allen, Tung, and Kaner 2010; Viculis, Mack, and Kaner 2003), Chemical Synthesis (Park and Rouff 2009), and thermal chemical vapour deposition (CVD) (Reina, Jia at al. 2009) synthesis are most commonly used methods. Some other techniques are also reported such as unzipping nano tube (Jiao et al. 2010; Kosynki et al. 2009; Jiao et al. 2009) and microwave synthesis (Xin et al. 2010); however those techinques need explored more extensively. There are numerous advantages ISSN 2686-5157

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to thermal CVD process. The process yields high quality and high purity final. products in large scale. Moreover, by controlling the CVD process parameters, control over the morphology, crystallinity, shape, and size of the desired product is possible.

In several investigation, Reina et al. demonstrated the formation of single-to few – layer graphene on polycrystalline Ni and transfer of graphene to any substrate by the wet-eching method (Reina, Jia, et al. 2009). They used e- beam evaporated Ni on a SiO2/Si substrate, annealed it at 900-1000 oC under flow of Ar and H2 for 10-20 minutes, followed by graphene growth using diluted hydrocarbon gas flow at 900-1000 oC and ambient pressure [5]. Ni-coated substrated are subjected to CVD growth at 900-1000 oC in flowing and highly dilute hydrocarbon (CH4/H2). The graphene film formed on the substrate was released by protecting the graphene film with poly(methyl methacrylate) (PMMA) and etching the underlying Ni with HCl aqueous solution (\approx 30% Vol.). there after, the film was transferred to substrate for analysis,

characterization, and application. The film are continuos over the entire area and can be patterned lithographically or by prepatterning the underlying catalytic Ni film. The optimal transmittance is approximately 90% in the 500 – 1000 nm wavelenght regime for a film having 3 nm average thickness, and resistance of the film are 770-1000 Ω /sq. The high instrintic quality of CVD graphene films makes them excellent candidates for both optoelectronic and electronic application. Rouff grup developed a large-scale graphene CVD growth process on the copper foils. The low solubility of carbon in copper appears to help make this growth process self limiting, and in agreement, the two- and three- layer flakes do not grow larger with the time. Compare to graphene growth on Ni, the films grow directly on the surface by a surface-catalized process rather than precipitation process. As a result, single-layer graphene, with only a small coverage of few layer, was formed predominantly across copper surface steps and grain boundaries. The graphene film formed on copper was released by iron etching of the copper subtrate and transferred to another substrate [6].

CVD/PV thin films are usually considered as coating having a thickness of less than ten microns. This is an arbitrary limitation and perhaps a better defenition would be a coating that adds little if any mass to substrate. A CVD reaction can occur in one of two basic systems: the closed reactor or open reactor (also known as close or open tube). The close-reactor system, also known as chemical transport, was the first type to be used for purification of metals. It is hybrid process which combines vapor-phase transfer with solid state diffusion. As the name implies, the chemicals are loaded in a container which is then tightly closed. A temperature differential is then applied which provides the driving force for reaction.

Open Reactor is the other CVD system is known as open-reactor of flowing-gas CVD, where the reactants are introduced continuously and flow through the reactor. Thermal CVD required high temperature, generally from 800 to 2000 oC, which can be generated by resistance heating, high-frequency induction, radiant heating, hot plate heating, or any combination of these. [7].

METODOLOGI

2.1.Method

The CVD design was conducted by ANSYS and HYSYS software. The purpose of chemical properties was simulated by HYSYS and ANSYS for pressure in capillary pipes.

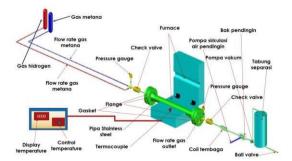


Figure 3.1 : CVD methane design

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RESULT AND DISCUSSION

3.1. Capillary Pipes Design by ANSYS

The design of capillary pipes CVD was drawn using the AUTOCAD dan simulated by ANSYS program. The materials of capillary was copper which have diameter about 0.25 mm.

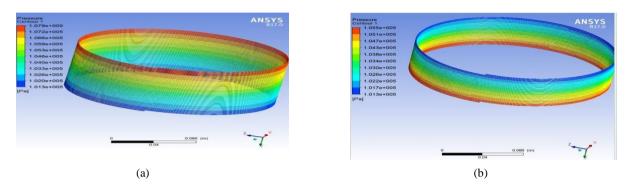


Figure 3.1: capillary pressure characteristics (a) capillary pipes 15 m (b) capillary pipes 25 m

ANSYS simulation results shown in Figures 3.1.a to 3.1.b shows that the resulting pressure at the length of the raw material gas output tube at the length of the cavity pipe with length 15 and 25 m respectively have an inlet and output pressure of 1.055 x 105 Pa, 1.013 x 105 Pa, 1.079 x 105 Pa, and 1.013 x 105 Pa. This investigations appear pressure fit as lower 1 atm at vaccum condition.

3.2. Process Condition of Energy Usage

Process energy is important for measure a balance between profit and product values. The efficiency of process was compared in reactor which operate at 4000 kJ and 4500 kJ.

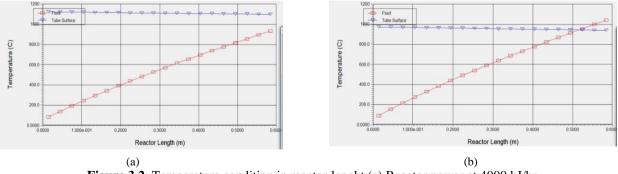


Figure 3.2: Temperature condition in reactor lenght (a) Reactor power at 4000 kJ/hr (b) Reactor power at 4500 kJ/hr.

Simulations were carried out using hysys 3.2. which aims to determine the effect of the power required to produce a reactor tube temperature and gas of at least 1000 oC. The tube reactor on the CVD has specifications (50 x 600 x 5) mm3 made of SS 316 material and a gas operating flowrate of 30 sccm in hydrogen gas and methane gas. In Figure 3.2.a It shows that in this condition the power given is 4000 kj / hour, indicating that the reactor tube **ISSN 2686-5157**

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reaches 1100 oC but at a length of 10 and 55 cm, the gas reaches 220 and 900 oC, respectively. Of course, these conditions have not yet reached the kinetic gas produced, but for the tube it is already in accordance with the conditions of 1100 oC. In Figure 3.2.b shows that in this condition the power given is 4500 kj / hour, indicating that the reactor tube reaches 1050 oC, then the conditions at 10 and 55 cm lengths, the gas reaches 220 and 1100 oC, respectively. These conditions indicate that the desired gas kinetic and tube temperature has reached the appropriate temperature so that it is predicted to form graphene.

3.3. Entalphy of CVD process

Reactor of CVD is formed reaction and result graphena. This Entalpy condition also refer to graphene formed.

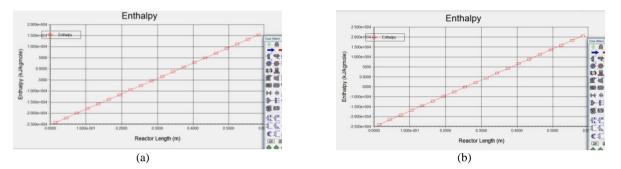


Figure 4.3 Entaphy in CVD reactor (a) entalphy condition at 4000 kJ/kg mole (b) entalphy condition at 4500 kJ/kg mole

Based on the research of Sun, X,. et al in 2018 stated that methane (C-H) and ethane gas had C-C energies ranging from 431 kJ/kg.mol and 368 kJ/kg.mol so that it can be stated in Figure 3.3.a. The energy for the formation of methyl radicals occurred at a length of 10 cm and the formation of graphene at a length of 45 cm tube. In Figure 4.3.a. It can be assumed that the energy of methyl radical formation occurs at a length of 10 cm and the formation of graphene at a tube length of 40 cm. In Figure 3.3.b. It can be assumed that the energy for the formation of methyl radicals occurs at a length of 10 cm and the formation of graphene at a length of 35 cm.

CONCLUSION

- 1. This simulations show that the CVD reactor have a minium power at 4500 kJ/hr and the pressure characteristics can be achieved use pipes diameter 0.25 mm was 1.013 x 105 Pa.
- 2. In entrophy cases shown methyl radical formation occurs at a length of 10 cm and the formation of graphene at a tube length of 40 cm.

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