Thermogravimetric Study of Dicyandiamide for Application in CVD Growth Process of Single Layer Film of Graphitic Carbon Nitride (g-C_3N_4)

Speaker: Michael M. Masaki, Abdul M. Syed, Caitlin M. Dragun-Bianchi, and Joel Therrien

University of Massachusetts Lowell (UML), Lowell, Massachusetts 01854, USA,

E-Mail: Michael_Masaki@student.uml.edu

Abstract

A well-characterized and controllable Chemical Vapor Deposition (CVD) based growth process for synthesis of single layer thin films of 2-D carbon-nitride (g-C_3N_4) based semiconductor materials is proposed. Since the discovery of graphene a decade ago there has been an immense interest in the study of 2-D materials beyond graphene in materials science applications, with focus on efficiency, low cost and environmentally friendly methods. Single layer g-C_3N_4 has a wide bandgap (~4.5 eV) and the potential to be enriched with carbon to form an alloy system bounded by g-C_3N_4 and graphene. CVD experiments to date have utilized a thermally decomposed solid source for growth of films, however this approach lacks a significant level of control and the gaseous reactant species are not well characterized. Here we will discuss the use of an easily accessible precursor, dicyandiamide (DiCy), which can be vaporized at low temperatures to achieve a controllable and well-characterized vapor source for the growth of g-C_3N_4. A thorough thermo-gravimetric study of DiCy, performed using a closed system for accessing mass loading and partial pressure of DiCy at various temperatures, along with supporting theoretical studies on single layer, few layer and multi-layer assemblies, and layered Van der Waals solids in general possessing remarkable electronic properties are presented. The initial experiment used sealed containers loaded with a quantity of DiCy. The containers were then heated to specified temperatures and held at these temperatures for about half-an hour to allow the entire system to reach equilibrium. The containers were then cooled and the change in mass of the DiCy was measured. DiCy that passed into vapor phase condensed on the container surface, resulting in a mass loss of the original sample, thus giving variance in mass loading of DiCy w.r.t temperatures ranging between 200°C – 210°C. This information can then be used to control the mass flow rate of DiCy introduced into a CVD reactor by an inert carrier gas, flowing over a solid DiCy sample held at a specific temperature. Such a proposed novel growth mechanism of single layer g-C_3N_4 using CVD system employing DiCy as a precursor, has opened a whole new era in exploiting the inherent optical band gap of g-C_3N_4 for post silicon electronic and optoelectronic devices. The importance of the mass loading curve, at specific temperatures for the precursor DiCy is discussed in detail.

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1. Professor Joel Therrien, Ph.D. Professor, Univ. of MA Lowell, ECE Department, Lowell, MA 01854.
2. UMass Lowell, ECE Dept., 1 University Ave., Ball Hall 301, Herbert J. Ball Eng. Center, Lowell, MA 01854.