Thermodynamic Analysis of Nanoscale PETN films

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Introduction

- Pentaerythritol Tetranitrate (PETN, C₅H₈N₄O₁₂) is one of the strongest secondary explosive commonly used as an initiator for other primary explosives
- Nanoscale measurements can provide methods of understanding and prohibiting coarsening
- No general agreement on thermal decomposition kinetics and determination of activation energy of evaporation of PETN

PETN powders (Lawrence Livermore National Laboratory, UC, California) dissolved in acetone (0.1M) and spin coated on to a piranha-cleaned Si(100) surface and dried in air
- PETN films are prepared by spin coating. (Single Wafer Spin Processor, Laurell Technologies Corp., North Wales, PA)
- Films were annealed isothermally (20-85°C) in oven (Isotemp Vacuum oven model 282A) at ambient pressures for 6 hours at each temperature
- The film was characterized after annealing at room temperature by AFM (Pacific Nanotechnology, Santa Clara, CA)
- PNI Nano-Rule+ software was used for measuring the volume and surface area of the coarsened region alone

State of the Art

Work that is presented is a continuation of an earlier work done by R. Pitchimani. Pitchimani’s work provided knowledge on the coarsening effects and speed of coarsening of PETN. This work will show how doping PETN will slow the coarsening effects by adding impurities.
- Zinc doped PETN has an increase in activation energy of sublimation thus stabilizing PETN at low temperatures.

Experimental

- Figure 1 shows the AFM image of the PETN film prepared at room temperature and the images after annealing for 12 hours each
- The AFM image taken 2 hours after preparation shows already some coarsening at some areas (brighter areas)
- The volume and the surface area of coarsened regions were measured at each temperature; The film vanishes at 70°C
- No general agreement on thermal decomposition kinetics and determination of activation energy of evaporation of PETN

Results (continued)

- Figure 2 shows the doped PETN films prepared at room temperature and the images annealed for 12 hours
- The film height increases continuously as the surface area increases up to about 60°C and then decreases. At and after 60°C the sublimation dominates
- Increased stability and decrease in coarsening effects shown from 55-65°C with Zn doped films
- Figure 3 shows the changes in activation energy of evaporation (Eₐ) with changes of doping levels
- We have determined the activation energy of evaporation (Eₐ) for PETN films of thickness few hundred nanometers in the temperature range 60-80°C
- The Eₐ values found for films match with that calculated for bulk PETN crystals in the temperature range 110-140°C
- The works extend the activation energy of evaporation for PETN in the lower temperature region
- Also using thin films for thermodynamic analysis of PETN makes it safer and can be extended to other explosives
- The work will be carried out with smaller temperature steps
- Impurities decrease coarsening effects

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References