Introduction: Silicon nanocrystals (SiNCs) with grain size less than 10 nm have been widely researched for its size-dependent optical and electronic properties [1]. It has been used as material for electronic devices such as hybrid solar cells, transistors and thermoelectric devices [2,3]. As for thermal properties, research on silicon nanocrystal showed promising result of adjustable thermal conductivity properties of silicon, by controlling the particle grain size [4]. Nanocomposite is mainly produced to increase the thermal conductivity of polymer based nanocomposite material. In contrast, in thermoelectric applications, overall thermal conductivity of nanocomposite material has to be reduced significantly while high electrical conductivity is maintained. Thermal conductivity is determined by the electron and phonon transport property of the composite materials, as shown in Fig. 1. Wang et al. reported the significant decrease of thermal conductivity with smaller silicon particles of 64 nm – 550 nm. Samples were prepared by mechanical pressing, followed by high-temperature annealing with more than 1200 °C [4].

In this work, nanocrystalline silicon particles with mean size of 6 nm were produced. In this case, NC size is much smaller than the phonon mean-free-path (MFP); therefore phonons experience significant number of scattering at the boundary, which is known as ballistic phonon transportation [4]. As a result, significant decrease of thermal conductivity is expected. Moreover, polymer forms nanostructured network where phonons also experience significant number of scattering at the NC/polymer interfaces: Thermal conductivity of the nanocomposite material is expected to decrease significantly. Additionally, with low temperature processes, unique size dependent property (quantum size effect) can be preserved and low cost fabrication is highly possible.

Experiment: SiNCs were synthesized by non-thermal plasma CVD [5]. Gas phase nucleation and growth occurred and excellent narrow size distribution with mean size of 6 nm nanocrystalline silicon particles were synthesized. As produced SiNCs were heated in ambient air at 200 °C for 12 hours to remove surface chlorine which forms silicon suboxide shell (SiOx). Samples were then thermal annealed at 800°C in N2 atmosphere (101 kPa) for 1 hour to form SiO2 shell. The core-shell structure would increase phonon scattering and confinement effects at the interfaces.

Results and discussion: Figure 2(a) and (b) show FTIR and Raman spectrum of SiNCs. Although SiNCs were heated in N2 atmosphere without oxygen, IR absorption spectrum shows the clear increase of Si-O-Si after thermal annealing. Correspondingly, Raman spectrum shows broad shoulder peak between 480-500 cm⁻¹. It indicates SiO2 is formed from suboxide shell (SiOx) under the lack of oxygen during annealing at 800°C, which may lead to the agglomeration of SiNCs and the formation of polycrystalline-like structure. Free-standing polystyrene (PS) thin film was fabricated by spin-casting as shown in Fig. 2(b) inset. Fabrication of SiNCs (6nm) and PS nanocomposite thin films with different weight ratio and their characterization will be presented in the conference.

References

![Figure 1 Schematic illustration of ballistic phonon transportation](image)

![Figure 2 (a) FTIR and (b) Raman spectrum of core-shell SiNCs with free-standing PS thin film (inset).](image)