ΣΕΜΙΝΑΡΙΟ

Observation of the Direct Energy Band Gaps of Defect Tolerant Cu_3N by Ultrafast Pump-Probe Spectroscopy

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Αίθουσα συνεδριάσεων
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(4ος όροφος του
κτιρίου της ΣΘΕ)

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Abstract

Cu_3N, Zn_3N_2 and Sn_3N_4 are earth abundant, metal nitrides, which are interesting from a fundamental and technological point of view but Cu_3N has been investigated in greater detail due to its unique properties that are attractive for energy conversion and storage. Cu_3N has a cubic a-ReO_3 crystal structure with a lattice constant of 3.8 Å and space group Pm3m, number 221. It is similar to the ABX_3 anti-perovskite structure with a vacant body-center position, so it can readily accommodate impurities and is a defect tolerant semiconductor. Here we show that Cu_3N with a cubic crystal structure can be prepared from Cu on fused SiO_2 under a flow of NH_3: O_2 between 400°C and 600°C. All Cu_3N layers exhibited distinct maxima in differential transmission at ~ 500 nm, 550 nm, and 630 nm, 670 nm with the same spectral structure and shape on an fs time scale as shown by ultrafast pump-probe spectroscopy. We show that the maxima at 630 nm (≡ 1.97 eV) and 670 nm (≡ 1.85 eV) correspond to the M and R direct energy band gaps of Cu_3N in excellent agreement with density functional theory calculations of the electronic band structure. In addition we suggest that the peaks at 500 nm (≡2.48 eV) and 550 nm (≡2.25 eV) most likely correspond to the M and R direct gap of certain regions of Cu_3N under strain that changes the lattice constant and band gap. We discuss the charge carrier generation and recombination mechanisms in terms of Cu interstitials and vacancies that are known to be energetically located near the band edges thus allowing the observation of the direct energy band gaps in this defect tolerant semiconductor. Finally we describe ongoing work on the synthesis and properties of Cu_3N nanoparticles prepared from Cu_2O nanoparticles.