



Materials

Making Ternary Quantum Dots From Single-Source Precursors

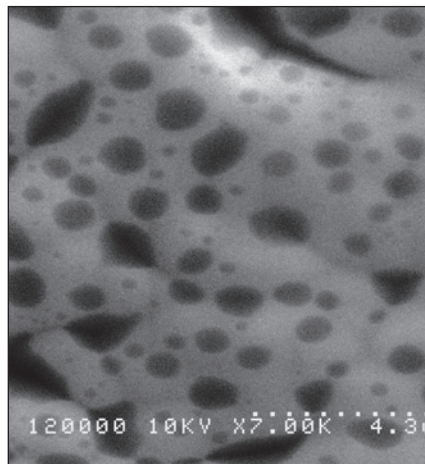
Relative to a prior process, this process is simpler and safer.

John H. Glenn Research Center, Cleveland, Ohio

A process has been devised for making ternary (specifically, CuInS_2) nanocrystals for use as quantum dots (QDs) in a contemplated next generation of high-efficiency solar photovoltaic cells. The process parameters can be chosen to tailor the sizes (and, thus, the absorption and emission spectra) of the QDs.

The process used heretofore to synthesize quantum dots in general involves *in situ* pyrolysis of reagents in the presence of a passivating solvent/ligand that not only serves as a medium for the formation of the QDs via pyrolysis, but also readily coordinates to the surfaces of the QDs, thereby preventing further nucleation. The prevention of further nucleation, also known as capping, serves to regulate the size of the QDs.

The present process is simpler and involves less handling of toxic reagents. Instead of the reagents of the prior process, one uses a compound of the type described in the first of the two immediately preceding articles, "Improved Single-Source Precursors for Solar-Cell Absorbers."



CuInS_2 Nanocrystals and Agglomerates on a polished silicon surface are shown in this scanning electron micrograph. The average diameter of the nanocrystals in this batch is 13.4 nm.

The single-source precursor is dissolved in trioctylphosphine under an inert atmosphere. The resulting solution is subsequently injected into a hot stirred so-

lution of trioctylphosphine oxide (TOPO) in order to facilitate controlled decomposition of the precursor to obtain the desired capped ternary quantum dots.

Aliquots of the solution are removed during the formation of the nanocrystals and are monitored via ultraviolet/visible-light spectroscopy to obtain information on the sizes of the nanocrystals. When the desired size range is reached, the reaction solution is cooled and methanol is added to remove excess precursor, leaving the TOPO-capped ternary nanocrystals to be harvested. The figure shows the product of one of several experiments performed to test this process.

This work was done by Sheila Bailey, Kulbinder Banger, Stephanie Castro, and Aloysius Hepp of Glenn Research Center. Further information is contained in a TSP (see page 1).

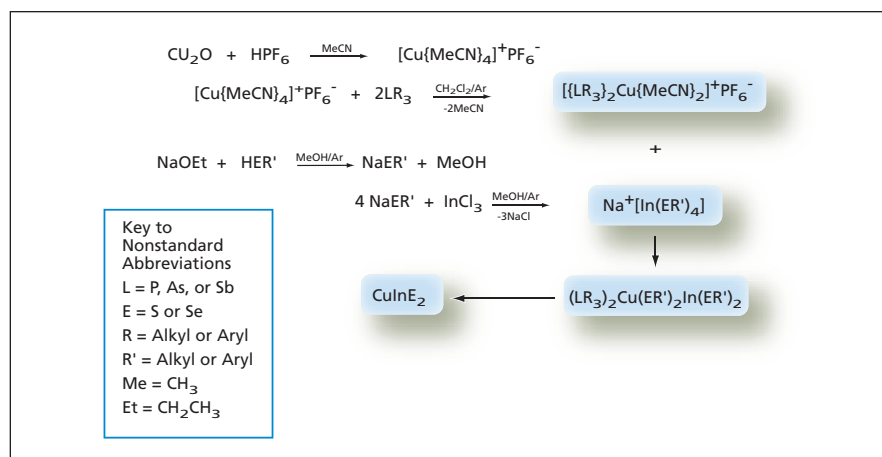
Inquiries concerning rights for the commercial use of this invention should be addressed to NASA Glenn Research Center, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-17446-1.

Improved Single-Source Precursors for Solar-Cell Absorbers

Deposition properties and final compositions can be tailored.

John H. Glenn Research Center, Cleveland, Ohio

Improved single-source precursor compounds have been invented for use in spray chemical vapor deposition (spray CVD) of chalcopyrite semiconductor absorber layers of thin-film solar photovoltaic cells. The semiconductors in question are denoted by the general formula $\text{CuIn}_x\text{Ga}_{1-x}\text{S}_y\text{Se}_{2-y}$, where $x \leq 1$ and $y \leq 2$. These semiconductors have been investigated intensively for use in solar cells because they exhibit long-term stability and a high degree of tolerance of radiation, and their bandgaps correlate well with the maximum photon power density in the solar spectrum. In addition, through selection of the proportions of Ga versus In and S versus Se, the bandgap of $\text{CuIn}_x\text{Ga}_{1-x}\text{S}_y\text{Se}_{2-y}$ can be tailored to a



These Sequences of Chemical Reactions are representative of the synthesis of a single-source precursor, in this case, $[(\text{LR}_3)_2\text{Cu}(\text{ER}')_2\text{M}(\text{ER}')_2]$ followed by formation of the chalcopyrite semiconductor (in this case, CuInE_2) from the precursor.