Argonne NATIONAL LABORATORY

News Release

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Compound could help detect chemical, biological weapons

Advanced Photon Source only place in U.S. to examine such small crystals

ARGONNE, Ill. (Sept. 26, 2008) – A light-transmitting compound that could one day be used in high-efficiency fiber optics and sensors that detect biological and chemical weapons at long distance almost went undiscovered by scientists because its structure was too difficult to examine.

Luckily, scientists from U.S. Department of Energy's Argonne National Laboratory and Northwestern University were able to determine the structure of the compound using the uniquely suited Chemistry and Materials (ChemMatCARS) beamline of the Center for Advanced Radiation Sources at the Advanced Photon Source.

"Like other such materials, this material has an electrically polarized structure," said Argonne scientist Mercouri Kanatzidis. "The incident light interacts with the electron cloud and in the process is disturbed. The disturbance changes the wavelength of the emitted light and creates two beams: the original and the second harmonic — a beam with half the wavelength and double the frequency."

This second-harmonic beam is 15 times more intense than that produced by the best current material. This two-for-one wavelength boost is paired with greater transparency, so the material can actually transmit the whole higher-wavelength beam.

These properties could have eventual real-world applications in identifying biological and chemical weapons at long distances and in optical communications.

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Compound – add one

However, these properties almost went undiscovered. The material, (A)$ZrPSe_{6,}$ where A can be potassium, rubidium or cesium, has a unique and difficult chemical structure that does not crystallize well. It grows lengthwise, but not in other directions. This creates long, thin crystals--perfect for fiber optics but a headache to study by conventional means.

"They are not very easy to design or make," Kanatzidis said. "It doesn't like to grow in other directions."

Finally, using the ChemMatCARS at the APS, Kanatzidis, Santanu Banerjee, Christos Malliakas, Joon I Jang, and John B. Ketterson were able to determine the structure and analyze its remarkable properties.

ChemMatCARS specializes in X-ray diffraction from ultra-small crystals and is operated by the University of Chicago.

A paper on their work can be seen in a recent edition of the Journal of the American Chemical Society *(J. Am. Chem. Soc. 2008, 37, 12270-12272.)*

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