Hard-X-Ray/Soft-γ-Ray Imaging Sensor Assembly for Astronomy
A pixilated scintillator is coupled with an array of avalanche photodiodes.

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An improved sensor assembly has been developed for astronomical imaging at photon energies ranging from 1 to 100 keV. The assembly includes a thallium-doped cesium iodide scintillator divided into pixels and coupled to an array of high-gain avalanche photodiodes (APDs). Optionally, the array of APDs can be operated without the scintillator to detect photons at energies below 15 keV. The array of APDs is connected to compact electronic readout circuitry that includes, among other things, 64 independent channels for detection of photons in various energy ranges, up to a maximum energy of 100

keV, at a count rate up to 3 kHz. The readout signals are digitized and processed by imaging software that performs "on-the-fly" analysis.

The sensor assembly has been integrated into an imaging spectrometer, along with a pair of coded apertures (Fresnel zone plates) that are used in conjunction with the pixel layout to implement a shadow-masking technique to obtain relatively high spatial resolution without having to use extremely small pixels. Angular resolutions of about 20 arc-seconds have been measured. Thus, for example, the imaging spectrometer can be used to (1) deter-

mine both the energy spectrum of a distant x-ray source and the angular deviation of the source from the nominal line of sight of an x-ray telescope in which the spectrometer is mounted or (2) study the spatial and temporal development of solar flares, repeating γ-ray bursters, and other phenomena that emit transient radiation in the hard-x-ray/soft-γ-ray region of the electromagnetic spectrum.

This work was done by Richard A. Myers of Radiation Monitoring Devices, Inc. for Goddard Space Flight Center. Further information is contained in a TSP (see page 1). GSC-14853-1

Simplified Modeling of Oxidation of Hydrocarbons
Only a few dozen molecular and radical species are included in calculations.

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A method of simplified computational modeling of oxidation of hydrocarbons is undergoing development. This is one of several developments needed to enable accurate computational simulation of turbulent, chemically reacting flows. At present, accurate computational simulation of such flows is difficult or impossible in most cases because (1) the numbers of grid points needed for adequate spatial resolution of turbulent flows in realistically complex geometries are beyond the capabilities of typical supercomputers now in use and (2) the combustion of typical hydrocarbons proceeds through decomposition into hundreds of molecular species interacting through thousands of reactions. Hence, the combination of detailed reaction-rate models with the fundamental flow equations yields flow models that are computationally prohibitive. Hence, further, a reduction of at least an order of magnitude in the dimension of reaction kinetics is one of the prerequisites for feasibility of computational simulation of turbulent, chemically reacting flows.

In the present method of simplified modeling, all molecular species involved

in the oxidation of hydrocarbons are classified as either light or heavy; heavy molecules are those having 3 or more carbon atoms. The light molecules are not subject to meaningful decomposition, and the heavy molecules are considered to decompose into only 13 specified constituent radicals, a few of which are listed in the table. One constructs a reduced-order model, suitable for use in estimating the release of heat and the evolution of temperature in combustion, from a base comprising the 13 constituent radicals plus a total of 26 other species that include the light molecules

and related light free radicals. Then rather than following all possible species through their reaction coordinates, one follows only the reduced set of reaction coordinates of the base.

The behavior of the base was examined in test computational simulations of the combustion of heptane in a stirred reactor at various initial pressures ranging from 0.1 to 6 MPa. Most of the simulations were performed for stoichiometric mixtures; some were performed for fuel/oxygen mole ratios of 1/2 and 2. The following are among the conclusions drawn from the results of these simulations:

Constituent Radical	δh^0	δh^c	δh^f
CH_3 (methyl)	−42.0	714	188
CH_2 (methylene)	−20.8	614.3	411
CH (methylidyne)	≈ −7	≈ 507	≈ 603
C_2H_3 (vinyl)	62.5	1,212	237

Some of the Constituent Radicals included in the simplified model are listed with some of their pertinent thermodynamic properties. The listed properties, all in units of kilojoules per mole, are the heat of formation (δh^0), the heat of combustion (δh^c), and the heat of component-to-free transition (δh^f). Other pertinent properties, omitted for the sake of simplicity, are coefficients in an equation for partial molar heat capacity as a function of temperature.

- The release of heat in combustion of heptane is modeled adequately.
- A simplified, low-dimensional chemistry model depends on an adequate representation of a reduced rate set. The net constituent rate is nearly quasi-steady and can be split into an incubation zone of modest temperature rise followed by a fast-reaction zone of high temperature.
- The incubation region is characterized by reaction times of the order of milliseconds — similar to diffusion time scales. Therefore, chemistry is expected to be significantly coupled with flow processes during incubation. This coupling gives rise to several issues that must be resolved in further development of a simplified model.
- In the fast-reaction zone, the coupling between chemistry and flow processes is weak, and combustion is determined primarily by the mixing rate. The temperature profiles in the fast-reaction zone tend to be independent of the details of behavior during incubation.

The development of the model is not yet complete. To close the model system of equations, it will be necessary to determine effective mean source strengths for light molecules and light radicals resulting from decomposition of heavy molecules. The final model will thus focus on reactions of the light species; the necessary rates are expected to be well determined insofar as kinetic interactions among light species prevail.

This work was done by Josette Bellan and Kenneth Harstad of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1). NPO-44750

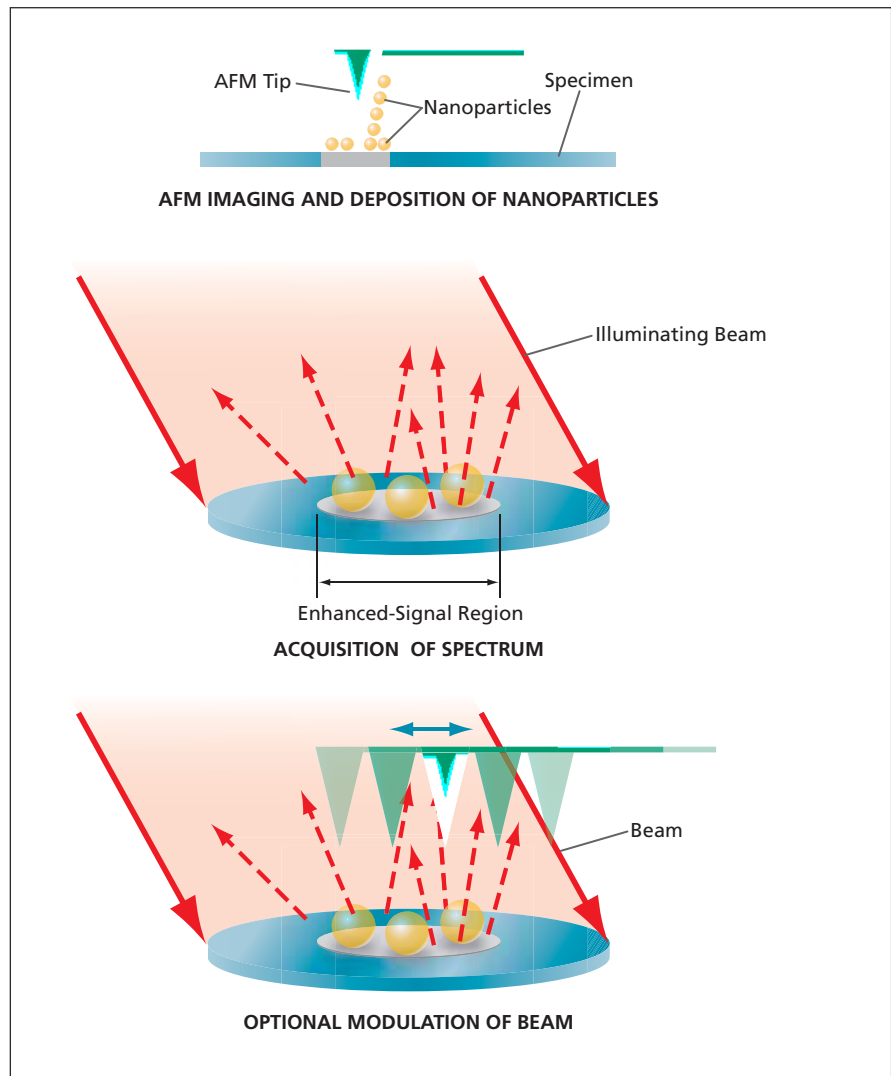# Near-Field Spectroscopy With Nanoparticles Deposited by AFM
It is not necessary to integrate an AFM with a spectrometer.

NASA's Jet Propulsion Laboratory, Pasadena, California

An alternative approach to apertureless near-field optical spectroscopy involving an atomic-force microscope (AFM) entails less complexity of equipment than does a prior approach. The alternative approach has been demonstrated to be applicable to apertureless near-field optical spectroscopy of the type using an AFM and surface enhanced Raman scattering (SERS), and is expected to be equally applicable in cases in which infrared or fluorescence spectroscopy is used.

Apertureless near-field optical spectroscopy is a means of performing spatially resolved analyses of chemical compositions of surface regions of nanostructured materials. In apertureless near-field spectroscopy, it is common practice to utilize nanostructured probe tips or nanoparticles (usually of gold) having shapes and dimensions chosen to exploit plasmon resonances so as to increase spectroscopic-signal strengths. To implement the particular prior approach to which the present approach is an alternative, it is necessary to integrate a Raman spectrometer with an AFM and to utilize a special SERS-active probe tip. The resulting instrumentation system is complex, and the tasks of designing and constructing the system and using the system to acquire spectro-chemical information from nanometer-scale regions on a surface are correspondingly demanding.

In the present alternative approach, unlike in the prior approach, one does not integrate a spectrometer with the AFM; that is, the spectrometer and the

AFM IMAGING AND DEPOSITION OF NANOPARTICLES

ACQUISITION OF SPECTRUM

OPTIONAL MODULATION OF BEAM

An **AFM Tip Is Used** to both image a specimen surface and deposit gold nanoparticles at a location of interest on the surface. Optionally, the tip can be moved through a spectrometer beam to modulate the light.