Shelton, CT, www.perkinelmer.com). Samples can be measured in reflectance mode or transmission mode. Solid samples such as biological tissues may need to be sliced into thin sections for transmission analysis. FTIR imaging can be performed on a wide variety of sample matrices, including polymers, pharmaceutical tablets, fibers, and coatings.

Commercial Raman and NIR imaging microscope systems are also available. Raman imaging of polymer blend surfaces, Raman and NIR imaging of silicon integrated circuits, and NIR imaging of whole pharmaceutical tablets are a few applications. The FALCON™ Raman Chemical Imaging Microscope (ChemIcon, Pittsburgh, PA, www.chemimage.com) can be equipped with fiber optic probes for remote monitoring and for high-temperature remote monitoring, such as in a heated process stream. The ChemIcon CONDOR™ Macro Chemical Imaging System can do NIR absorption imaging as well as fluorescence and visible emission imaging. A fast near-IR Raman Imaging microscope system (NIRIM) is described by McLain and coauthors that uses a fiber optic bundle and CCD detector to collect a complete 3D Raman data cube from a sample in 1 s or less. A schematic of the NIRIM is shown in Fig. 4.76. The system has been used to image inorganic inclusions in crystals, mixtures of metal oxides, amino acid mixtures and to perform surface-enhanced Raman imaging of catalyst and nanoparticle surfaces, among other studies. Two examples are shown in Figs. 4.77 and 4.78.

Chemical imaging provides a nondestructive and noninvasive way to map the chemical composition of a wide variety of samples very rapidly and at the microscopic

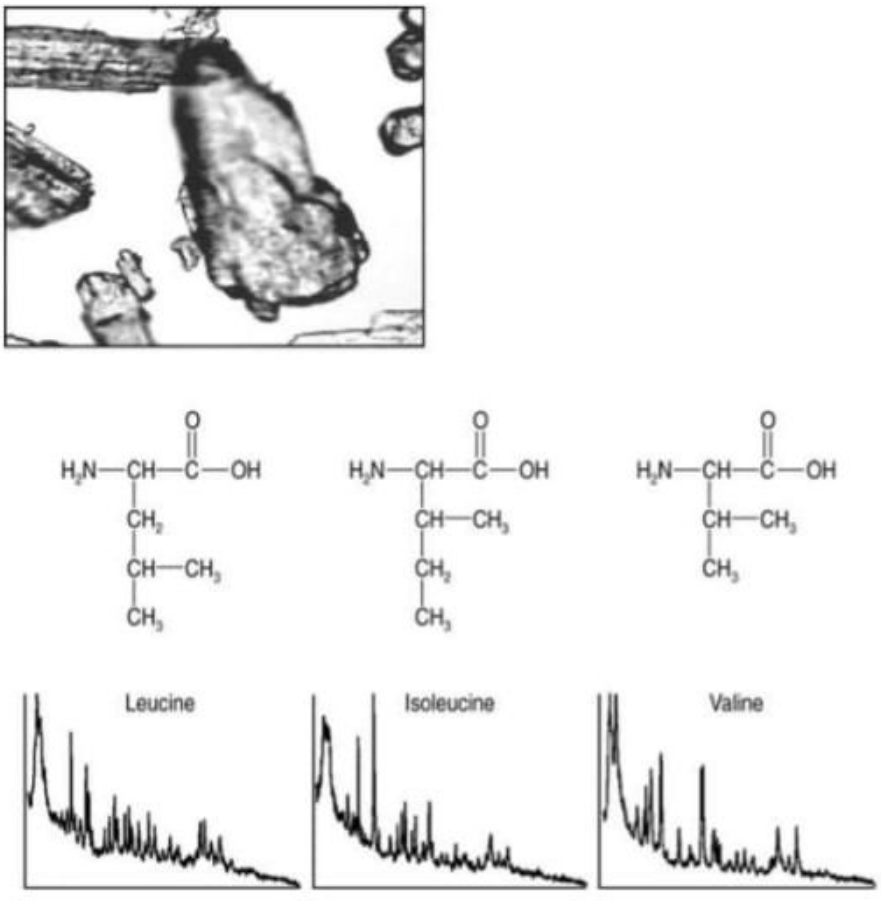

Figure 4.78 Imaging and identification of three different amino acid crystals in a mixture using the NIRIM system. (Reprinted from McLain et al., with permission from Advanstar Communications, Inc.)

4.9. CHEMICAL IMAGING USING NIR, IR, AND RAMAN SPECTROSCOPY

The most recent breakthrough in the use of vibrational spectroscopy for chemical analysis is in the area of *chemical imaging*. Chemical imaging is the use of 2D or 3D detectors to collect spectral data from a large number of locations within a sample and then using the variations in the spectral data to map chemical differences within the sample. The chemical differences are often displayed as a false-color image of the sample. The use of chemical imaging technology in NMR has been described in Chapter 3; it is the technique more commonly called MRI.

FTIR imaging has been commercially available since 1996. The usual "detector" is an MCT array detector, called a focal plane array (FPA) detector, used in conjunction with an FTIR microscope. A 64 × 64 FPA detector has 4096 detector elements and allows 4096 interferograms to be collected simultaneously. Because each pixel in the detector array generates a spectrum, there are three dimensions in the data set. These data sets are often referred to as data cubes or image cubes. The x and y coordinates of the cube are the spatial positions while the z coordinate represents the wavelength, as shown in Fig. 4.74. The data can be handled in many ways, including the use of library searching, principal component analysis, and more, making this a powerful technique. As a simple example, the intensity of the carbonyl-stretching band in each pixel can be "reassembled" into the visual image seen through the microscope, giving a distribution of carbonyl-containing material in the sample. Such an image is shown in Fig. 4.75, collected with the Spectrum Spotlight 300 FTIR Imaging System (PerkinElmer Instruments,

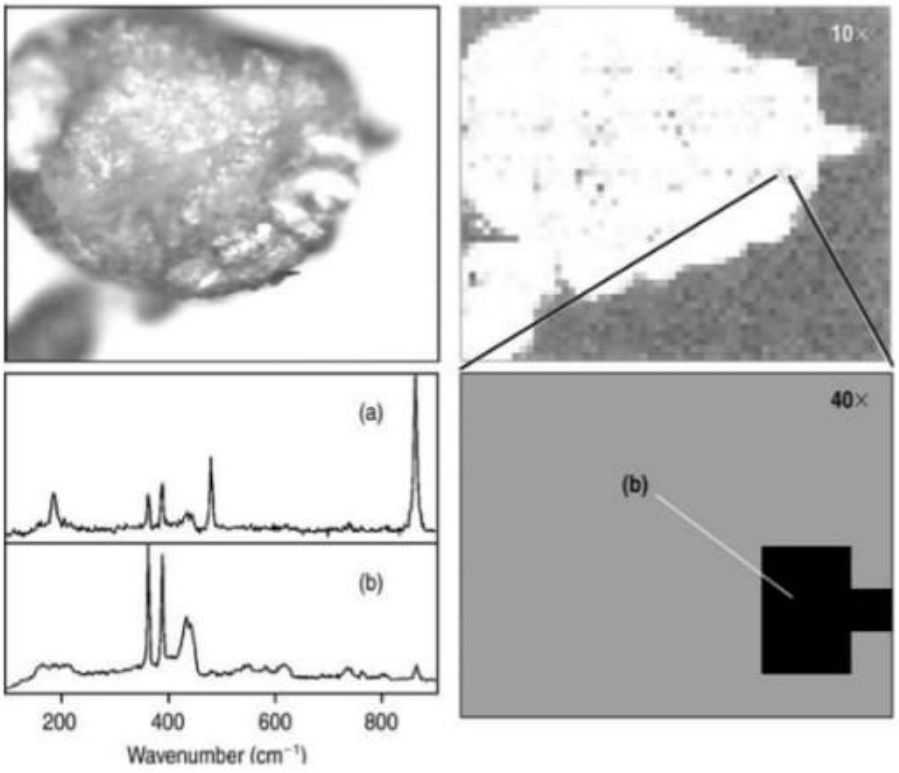

Figure 4.77 Identification of a small molybdenum sulfide inclusion in a larger boric acid crystal using the NIRIM system. (Reprinted from McLain et al., with permission from Advanstar Communications, Inc.)