

directed through a hole in the center of a parabolic mirror **184** towards the inlet orifice **183** of the mass spectrometer, as shown in **FIG. 17**. A laser beam from a laser **181** is directed at and reflected from the mirror **182** so that the light beam is collinear with the droplet beam. Laser **181** wavelength is chosen for optimal absorption by the solvent to cause evaporation, and a long interaction length between drop stream **185** and the laser beam allows the use of a low power laser **181**. Optimization of the laser power, wavelength and characteristics of piezo-electric droplet dispensing can allow for a complete evaporation of solvent from the droplets **185**. Sample ionization may be achieved by applying an electrical potential to the gold plated parabolic mirror **184** through which the droplets **185** are fired. Alternatively, an atmospheric pressure chemical ionization scheme can be used to ionize samples.

#### [0098] Rapid Heating

[0099] **FIG. 18** is a schematic diagram of a system **194** for rapidly heating samples on a moving surface **192** so as to cause atomization, in accordance with one embodiment of the invention. A sample is atomized and directed at the inlet orifice **191** of an analyzer by rapidly heating a small amount of the sample in an enclosed volume **193** with a narrow channel from which it can be released. The sample reservoir **193** may either be incorporated directly into the belt itself, or the samples could be transferred from the belt into reservoirs on a separate instrument. The geometry and structure of the exit channel from the sample reservoir **193** can be designed such that upon rapid heating of the reservoir the natural expansion of the sample cause it to be ejected from the reservoir through the orifice in the form of an atomized spray. This spray is analogous to ESI-MS and can be directed at the inlet orifice of the mass spectrometer. The geometry and shape of the reservoir **193** and exit channel with respect to the MS inlet orifice **191**, the mass spectrometer inlet temperature, and the flow rate and character of the sheath gas can be optimized to provide the largest amount of atomization. Sample ionization can be accomplished by chemical ionization by increasing the partial pressure of a gas such as methane or ammonia near the atomized sample and by introducing the gas and sample to a corona discharge needle. This approach is similar to that used in atmospheric pressure chemical ionization (APCI-MS) schemes.

[0100] The heating of the reservoir can be accomplished either thermoelectrically or by focusing a laser beam inside the sample within the reservoir.

#### [0101] Pneumatic or Explosive Force

[0102] **FIG. 19** is a schematic diagram of a system **2006** for forcibly ejecting a sample from a moving surface **2005**, in accordance with one embodiment of the invention. A sample is placed within a reservoir **2002** with the appropriate geometry such that if forcefully ejected from reservoir **2002** the sample will atomize into a fine spray. If desired, the sample can be ejected from the reservoir through a narrow channel to increase the amount of sample that is atomized. Reservoirs **2002** may either be built directly into moving surface **2005** or samples can be transferred from moving surface **2005** to a separate instrument containing reservoirs **2002**. Reservoir **2002** is positioned with a geometry such that when the sample is ejected from reservoir **2002** it is atomized and directed at the analyzer, for example, at the inlet orifice **2004** of the mass spectrometer. Reservoir **2002**

may be shaped such that the atomization process is optimized. The sample may either be ejected with the use of a small explosive charge or by a pneumatic piston **2001** that actuates and applies pressure on the bottom of reservoir **2002**. The geometry and shape of reservoir **2002** and exit channel with respect to the MS inlet orifice, mass spectrometer inlet **2004** temperature, and the flow rate and character of the sheath gas may be optimized to provide the desired amount of sample atomization and MS signal. Ionization of the sample may be performed by the use of an ionization gas such as methane or ammonia and a corona discharge needle **2003** similar to APCI-MS.

#### [0103] Vibration

[0104] **FIG. 20** is a schematic diagram of a system **2106** for rapidly vibrating samples on a moving surface **2101** so as to cause atomization, in accordance with one embodiment of the invention. A liquid sample **2104** deposited on a thin surface **2101** is atomized by rapid vibration of that surface **2101**. The surface **2101** onto which the sample is deposited may be a thin film, such as the moving surface itself, or alternatively, the sample can be transferred to a suitable surface such as a thin film with a surface coating, a narrow flexible strip, or the point of a pin or needle. The rapid vibration of the sample **2104** may be performed by focusing a pulsed laser onto the surface near the sample **2104**, or onto the backside of the surface onto which the sample has been deposited. Alternatively, acoustic systems using ultrasonic waves or a rapid mechanical system can be used to generate vibration. The sample may also be made to vibrate by using an alternating current **2201** to cause a probe **2203** onto which the sample **2204** has been deposited to move rapidly back and forth, as shown in **FIG. 21**. In this embodiment, the vibrating device **2206** is similar to the probe of an atomic force microscope (AFM), where the sample is deposited onto the tip of a probe similar to that of an AFM and rapid vibration of the probe results in atomization of that sample. In accordance with various embodiments of the invention, the surface onto which the sample is deposited can be made hydrophilic or hydrophobic, and the temperature of the surface and mass spectrometer inlet **2103**, **2202** and the geometry and flow rate of the sheath gas can be optimized to provide the best sample atomization. Additionally, a voltage may be applied to the surface onto which the sample is deposited to assist in the formation of an appropriate spray for mass spectrometer interfacing. If desired, ionization of the sample can be performed by the use of a chemical ionization gas such as methane or ammonia and a corona discharge needle **2102**, **2205** similar to APCI-MS.

#### [0105] High Throughput Screening Software Architecture

[0106] In accordance with one embodiment of the invention, the high throughput processing system architecture may be conceptually divided into two basic functional layers organized as a hierarchical relationship between subordinate task orientated components and a supervisory component which manages the coordination of the subordinate tasks, as shown in **FIG. 22**. In **FIG. 22**, relationships between the system architecture elements are shown with lines indicating the flow of data between elements. Each component represents an independently running thread of execution or an entirely separate process, which may run on separate processors where desired. This is an important characteristic that is emphasized in order to highlight the flexibility and