Vaporization processes are an important alternative to plasma-aided deposition methods, especially with sensitive substrates and precursors which could be damaged in plasma processes by highly energized particles. Vaporization processes are used among other things in web coating, in coating sensitive semiconductor structures or in the vaporization of organic precursors, for OLED displays. Vapor deposition on large areas with good coating homogeneity is a challenge. For this reason the Fraunhofer IST offers the possibility of modeling the vaporization process in the sense of model-supported source development.

**Modeling of vaporization processes**

One special aspect in modeling vaporization processes is the wide pressure range which must be taken into consideration. While in most cases there is still laminar flow at the vaporizer source, the pressure drops rapidly even a small distance away, which means that there is a transition to molecular flow. These kind of flow cases are no more properly represented in continuum dynamics based on Navier-Stokes equation, instead the more generalized Boltzmann transport equation is required. For this purpose Fraunhofer IST has developed a software for solving the Boltzmann equation via Direct Simulation Monte Carlo (DSMC) method on a statistical basis. Thanks to parallelization even large and complex problems can be processed.

By way of example let us present a 2D simulation of the aluminum vaporization of four adjacent linear sources. The source width and the distance between the sources in each case measure 100 mm and at a distance of 800 mm from the sources there is a substrate 2 m wide. As can be seen from the aluminum pressure profile shown in Fig. 1, the collision events between the vaporized aluminum atoms result in complex dynamic interactions close to the source. At a high vapor pressure these lead to detectable features in the resulting coating thickness profile (see graph).

**Outlook**

Advanced techniques such as multiphase vaporization processes bear even more complex interactions. Fraunhofer IST offers to support the development of advanced vaporization processes by means of simulation-based optimization studies.
Simulated pressure profile in aluminum vaporization from four linear sources at a vapor pressure of 1 mbar.