

## VA 4: Diffusion, magnetic thin films

Time: Monday 15:30–16:10

Location: HSZ 101

VA 4.1 Mon 15:30 HSZ 101

**Simulation of Diffusion Processes in Rarefied Gases - A Hybrid Approach** — DAVID SINZ<sup>1,2</sup>, ●JENS HARTING<sup>1</sup>, FRANZ KELLER<sup>2</sup>, and ULRICH NIEKEN<sup>2</sup> — <sup>1</sup>Institut für Computerphysik, Pfaffenwaldring 27, 70569 Stuttgart — <sup>2</sup>Institut für Chemische Verfahrenstechnik, Böblinger Str. 72, 70199 Stuttgart

We simulate diffusion-convection problems in rarefied gases in order to predict the diffusive spreading of low concentrated contaminants in a stream of purge gas.

The proposed simulation method is a hybrid approach combining the lattice Boltzmann method (LBM) and a simplified molecular dynamics (MD) approach. Here, the flow field of the purge gas is simulated using the LBM and the behaviour of the contaminants is described by a MD approach neglecting the interaction of the particles with each other and the gas. The influence of the purge gas on the contaminants is modeled by central collisions with pseudo particles, where the collision frequency depends on the mean free path of the MD particles. The velocity of the pseudo particles is determined by the predicted flow field of the purge gas as well as thermal fluctuations.

Our approach requires substantially less computing time than a regular MD approach and allows the simulation of systems of technically interesting dimensions. The method is evaluated by comparing simulation results to analytical solutions for simple test cases as well as to experimental data for a more complex case both with acceptable agreement.

VA 4.2 Mon 15:50 HSZ 101

**Spin-resolved HAXPES technique for the investigation of new spintronic materials.** — ●GREGORY STRYGANYUK<sup>1</sup>, SIHAM QUARDI<sup>1</sup>, XENIYA KOZINA<sup>1</sup>, ANDREI GLOSKOVSKII<sup>1</sup>, GERHARD H. FECHER<sup>1</sup>, CLAUDIA FELSER<sup>1</sup>, MICHAELA HAHN<sup>2</sup>, GERD SCHÖNHENSE<sup>2</sup>, MASAFUMI YAMAMOTO<sup>3</sup>, KOICHIRO INOMATA<sup>4</sup>, ELJI IKENAGA<sup>5</sup>, and KEISUKE KOBAYASHI<sup>5</sup> — <sup>1</sup>Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55128 Mainz — <sup>2</sup>Institute of Physics, Johannes Gutenberg - University, 55128 Mainz — <sup>3</sup>Graduate School of Information Science and Technology, Hokkaido University, Sapporo, Japan — <sup>4</sup>National Institute for Materials Science, Tsukuba 305-0047, Japan — <sup>5</sup>SPring-8 JASRI, Hyogo, 679-5198, Japan

The elaboration of innovative spintronic devices implies the employment of spin dependent electronic properties of magnetic materials. Growing interest in search and development of promising spintronic materials requires spin-resolved studies. This work reports on the development of spin polarized high resolution hard X-ray photoemission spectroscopy (SPIN HAXPES) at SPring-8. Hard X-ray excitation provides the possibility to study a whole spintronic multilayer device due to the large inelastic mean free path of the photoelectrons at high kinetic energies. The implementation of SPIN HAXPES using a SCIENTA R4000 analyzer equipped with SPLEED detector is discussed. The installation of a phase retarder at BL47XU beamline is considered for studies of magnetic circular dichroism in the core level photoemission and spin-resolved experiments. This work is funded by JST-DfG (Project FE 633/6-1).